



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 03:41 pm GMT

PDB ID : 6FKR  
Title : Crystal structure of the dolphin proline-rich antimicrobial peptide Tur1A bound to the *Thermus thermophilus* 70S ribosome  
Authors : Mardirossian, M.; Perebaskine, N.; Benincasa, M.; Gambato, S.; Hofmann, S.; Huter, P.; Muller, C.; Hilpert, K.; Innis, C.A.; Tossi, A.; Wilson, D.N.  
Deposited on : 2018-01-24  
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

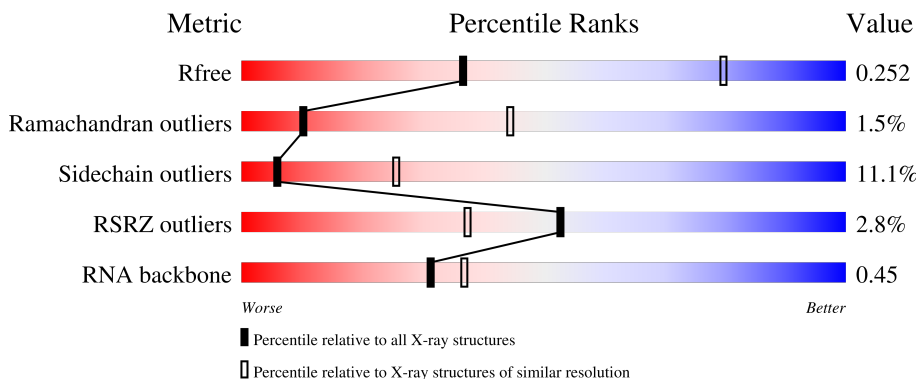
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2901	
1	2A	2901	
2	1B	120	
2	2B	120	
3	1D	275	

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Mol	Chain	Length	Quality of chain
3	2D	275	90% 9%
4	1E	204	84% 15%
4	2E	204	89% 11%
5	1F	203	85% 15%
5	2F	203	89% 11%
6	1G	181	88% 9%
6	2G	181	90% 9%
7	1H	174	94% 6%
7	2H	174	93% 7%
8	1I	147	81% 18%
8	2I	147	82% 17%
9	1N	140	86% 14%
9	2N	140	88% 12%
10	1O	122	91% 7%
10	2O	122	92% 7%
11	1P	149	91% 8%
11	2P	149	90% 9%
12	1Q	141	90% 10%
12	2Q	141	90% 9%
13	1R	118	80% 19%
13	2R	118	87% 12%
14	1S	110	86% 14%
14	2S	110	89% 11%
15	1T	131	89% 10%
15	2T	131	92% 8%

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Mol	Chain	Length	Quality of chain
16	1U	116	84% 16%
16	2U	116	89% 11%
17	1V	101	86% 14%
17	2V	101	92% 8%
18	1W	112	88% 12%
18	2W	112	86% 14%
19	1X	95	95% 5%
19	2X	95	94% 6%
20	1Y	107	87% 13%
20	2Y	107	88% 12%
21	1Z	203	89% 10%
21	2Z	203	89% 11%
22	10	77	95% 5%
22	20	77	95% 5%
23	11	97	92% 8%
23	21	97	95%
24	12	70	90% 10%
24	22	70	93% 6%
25	13	59	80% 19%
25	23	59	86% 14%
26	14	69	81% 17%
26	24	69	81% 19%
27	15	59	86% 14%
27	25	59	88% 12%
28	16	53	85% 15%

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Mol	Chain	Length	Quality of chain
28	26	53	91% 9%
29	17	48	83% 15%
29	27	48	2% 85% 15%
30	18	64	89% 11%
30	28	64	92% 8%
31	19	37	86% 14%
31	29	37	8% 89% 11%
32	1a	1507	2% 58% 36% 5%
32	2a	1507	2% 62% 32% 6%
33	1b	231	3% 82% 16%
33	2b	231	3% 81% 18%
34	1c	206	2% 91% 9%
34	2c	206	5% 93% 6%
35	1d	208	84% 15%
35	2d	208	87% 12%
36	1e	148	93% 7%
36	2e	148	91% 9%
37	1f	100	92% 8%
37	2f	100	94% 6%
38	1g	155	3% 92% 8%
38	2g	155	10% 93% 6%
39	1h	137	93% 7%
39	2h	137	93% 7%
40	1i	127	6% 84% 15%
40	2i	127	11% 87% 12%

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Mol	Chain	Length	Quality of chain
41	1j	97	12% 92% 7%
41	2j	97	15% 89% 11%
42	1k	114	95% 5%
42	2k	114	2% 92% 8%
43	1l	122	% 93% 7%
43	2l	122	93% 7%
44	1m	116	5% 92% 7%
44	2m	116	11% 91% 6%
45	1n	60	3% 87% 13%
45	2n	60	8% 88% 12%
46	1o	88	% 94% 6%
46	2o	88	95% 5%
47	1p	82	4% 80% 20%
47	2p	82	4% 83% 17%
48	1q	99	% 91% 9%
48	2q	99	92% 8%
49	1r	68	90% 10%
49	2r	68	3% 90% 10%
50	1s	83	11% 90% 8%
50	2s	83	39% 90% 10%
51	1t	96	2% 90% 8%
51	2t	96	% 91% 7%
52	1u	23	13% 87% 13%
52	2u	23	61% 91% 9%
53	1y	22	5% 50% 50%

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Mol	Chain	Length	Quality of chain
54	1z	97	<p>97%</p>
54	2z	97	<p>98%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	1A	3032	-	-	-	X
55	MG	1A	3040	-	-	-	X
55	MG	1A	3048	-	-	-	X
55	MG	1A	3074	-	-	-	X
55	MG	1A	3081	-	-	-	X
55	MG	1A	3085	-	-	-	X
55	MG	1A	3122	-	-	-	X
55	MG	1A	3173	-	-	-	X
55	MG	1A	3184	-	-	-	X
55	MG	1A	3253	-	-	-	X
55	MG	1A	3480	-	-	-	X
55	MG	1A	3493	-	-	-	X
55	MG	1A	3528	-	-	-	X
55	MG	1A	3553	-	-	-	X
55	MG	1A	3562	-	-	-	X
55	MG	1A	3584	-	-	-	X
55	MG	1A	3602	-	-	-	X
55	MG	1A	3638	-	-	-	X
55	MG	1A	3650	-	-	-	X
55	MG	1A	3717	-	-	-	X
55	MG	1A	3780	-	-	-	X
55	MG	1A	3912	-	-	-	X
55	MG	1A	3946	-	-	-	X
55	MG	1A	3957	-	-	-	X
55	MG	1B	217	-	-	-	X
55	MG	1Q	203	-	-	-	X
55	MG	1X	102	-	-	-	X
55	MG	1a	1632	-	-	-	X
55	MG	1a	1640	-	-	-	X
55	MG	1a	1644	-	-	-	X
55	MG	1a	1661	-	-	-	X
55	MG	1a	1666	-	-	-	X
55	MG	1a	1669	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	1a	1676	-	-	-	X
55	MG	1a	1680	-	-	-	X
55	MG	1a	1684	-	-	-	X
55	MG	1a	1770	-	-	-	X
55	MG	1a	1806	-	-	-	X
55	MG	1a	1835	-	-	-	X
55	MG	1d	303	-	-	-	X
55	MG	23	102	-	-	-	X
55	MG	29	101	-	-	-	X
55	MG	29	104	-	-	-	X
55	MG	2A	3022	-	-	-	X
55	MG	2A	3025	-	-	-	X
55	MG	2A	3051	-	-	-	X
55	MG	2A	3098	-	-	-	X
55	MG	2A	3109	-	-	-	X
55	MG	2A	3116	-	-	-	X
55	MG	2A	3152	-	-	-	X
55	MG	2A	3164	-	-	-	X
55	MG	2A	3176	-	-	-	X
55	MG	2A	3177	-	-	-	X
55	MG	2A	3187	-	-	-	X
55	MG	2A	3194	-	-	-	X
55	MG	2A	3199	-	-	-	X
55	MG	2A	3202	-	-	-	X
55	MG	2A	3230	-	-	-	X
55	MG	2A	3232	-	-	-	X
55	MG	2A	3250	-	-	-	X
55	MG	2A	3279	-	-	-	X
55	MG	2A	3404	-	-	-	X
55	MG	2A	3413	-	-	-	X
55	MG	2A	3419	-	-	-	X
55	MG	2A	3559	-	-	-	X
55	MG	2A	3591	-	-	-	X
55	MG	2A	3594	-	-	-	X
55	MG	2A	3599	-	-	-	X
55	MG	2A	3641	-	-	-	X
55	MG	2A	3644	-	-	-	X
55	MG	2A	3650	-	-	-	X
55	MG	2A	3694	-	-	-	X
55	MG	2A	3720	-	-	-	X
55	MG	2A	3727	-	-	-	X
55	MG	2A	3751	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	2A	3753	-	-	-	X
55	MG	2A	3764	-	-	-	X
55	MG	2A	3781	-	-	-	X
55	MG	2A	3782	-	-	-	X
55	MG	2A	3784	-	-	-	X
55	MG	2A	3795	-	-	-	X
55	MG	2A	3800	-	-	-	X
55	MG	2A	3819	-	-	-	X
55	MG	2A	3907	-	-	-	X
55	MG	2A	3911	-	-	-	X
55	MG	2A	3915	-	-	-	X
55	MG	2A	3929	-	-	-	X
55	MG	2A	3931	-	-	-	X
55	MG	2A	3939	-	-	-	X
55	MG	2A	3941	-	-	-	X
55	MG	2A	3944	-	-	-	X
55	MG	2A	3945	-	-	-	X
55	MG	2A	3969	-	-	-	X
55	MG	2B	3008	-	-	-	X
55	MG	2B	3009	-	-	-	X
55	MG	2B	3014	-	-	-	X
55	MG	2B	3016	-	-	-	X
55	MG	2B	3026	-	-	-	X
55	MG	2D	308	-	-	-	X
55	MG	2F	310	-	-	-	X
55	MG	2H	8001	-	-	-	X
55	MG	2Y	201	-	-	-	X
55	MG	2a	1617	-	-	-	X
55	MG	2a	1619	-	-	-	X
55	MG	2a	1624	-	-	-	X
55	MG	2a	1631	-	-	-	X
55	MG	2a	1635	-	-	-	X
55	MG	2a	1639	-	-	-	X
55	MG	2a	1640	-	-	-	X
55	MG	2a	1643	-	-	-	X
55	MG	2a	1651	-	-	-	X
55	MG	2a	1663	-	-	-	X
55	MG	2a	1665	-	-	-	X
55	MG	2a	1668	-	-	-	X
55	MG	2a	1672	-	-	-	X
55	MG	2a	1796	-	-	-	X
55	MG	2a	1827	-	-	-	X

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
55	MG	2a	1828	-	-	-	X
55	MG	2a	1834	-	-	-	X
55	MG	2d	504	-	-	-	X
55	MG	2i	3001	-	-	-	X
55	MG	2z	101	-	-	-	X

## 2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 294294 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1A	2872	Total	C	N	O	P	0	0	0
			61872	27540	11574	19886	2872			
1	2A	2872	Total	C	N	O	P	0	0	0
			61872	27540	11574	19886	2872			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1A	652R	G	C	conflict	GB 37223181
1A	1227	G	UNK	conflict	GB 37223181
2A	652R	G	C	conflict	GB 37223181
2A	1227	G	UNK	conflict	GB 37223181

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	1B	120	Total	C	N	O	P	0	0	0
			2575	1145	476	834	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1145	476	834	120			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	1D	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	2E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	2N	140	1121	722	208	187	4	0	0	0

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	1O	122	933	588	171	170	4	0	0	0
10	2O	122	933	588	171	170	4	0	0	0

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	1P	149	1135	706	230	196	3	0	0	0
11	2P	149	1135	706	230	196	3	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	1Q	141	1122	715	212	188	7	0	0	0
12	2Q	141	1122	715	212	188	7	0	0	0

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	1R	118	968	604	203	160	1	0	0	0
13	2R	118	968	604	203	160	1	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	1S	110	877	553	175	149	0	0	0
14	2S	110	877	553	175	149	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	1T	131	Total 1091	C 680	N 225	O 185	S 1	0	0	0
15	2T	131	Total 1091	C 680	N 225	O 185	S 1	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	1U	116	Total 959	C 608	N 201	O 149	S 1	0	0	0
16	2U	116	Total 959	C 608	N 201	O 149	S 1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	1V	101	Total 775	C 498	N 141	O 135	S 1	0	0	0
17	2V	101	Total 775	C 498	N 141	O 135	S 1	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	1W	112	Total 886	C 557	N 174	O 153	S 2	0	0	0
18	2W	112	Total 886	C 557	N 174	O 153	S 2	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	1X	95	Total 750	C 488	N 135	O 126	S 1	0	0	0
19	2X	95	Total 750	C 488	N 135	O 126	S 1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	13	59	Total	C	N	O	0	0	0
			469	298	90	81			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
25	23	59	469	298	90	81	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	14	69	546	346	96	99	5	0	0	0
26	24	69	546	346	96	99	5	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	15	59	459	288	90	76	5	0	0	0
27	25	59	459	288	90	76	5	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	16	53	453	281	91	77	4	0	0	0
28	26	53	453	281	91	77	4	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	17	48	418	257	104	55	2	0	0	0
29	27	48	418	257	104	55	2	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	18	64	517	331	102	82	2	0	0	0
30	28	64	517	331	102	82	2	0	0	0



- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	19	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
31	29	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called 16 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
37	2f	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			986	625	193	168			
40	2i	127	Total	C	N	O	0	0	0
			986	625	193	168			

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			719	446	142	131			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	2j	97	Total	C	N	O	0	0	0
			719	446	142	131			

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			
42	2k	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	1l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			
43	2l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	2m	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	1o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
46	2o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	1p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
47	2p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
48	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	1r	68	Total	C	N	O	0	0	0
			555	355	108	92			
49	2r	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
51	2t	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			

- Molecule 52 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a protein called Tur1A peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	1y	22	Total	C	N	O	0	0	0
			168	111	34	23			

- Molecule 54 is a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1z	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			
54	2z	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1A	957	Total	Mg	0	0
			957	957		
55	1B	28	Total	Mg	0	0
			28	28		
55	1D	17	Total	Mg	0	0
			17	17		
55	1E	5	Total	Mg	0	0
			5	5		
55	1F	14	Total	Mg	0	0
			14	14		
55	1G	3	Total	Mg	0	0
			3	3		
55	1H	2	Total	Mg	0	0
			2	2		
55	1N	4	Total	Mg	0	0
			4	4		
55	1P	4	Total	Mg	0	0
			4	4		
55	1Q	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1R	4	Total Mg 4 4	0	0
55	1T	2	Total Mg 2 2	0	0
55	1U	5	Total Mg 5 5	0	0
55	1V	3	Total Mg 3 3	0	0
55	1W	3	Total Mg 3 3	0	0
55	1X	2	Total Mg 2 2	0	0
55	1Y	1	Total Mg 1 1	0	0
55	10	7	Total Mg 7 7	0	0
55	11	4	Total Mg 4 4	0	0
55	13	2	Total Mg 2 2	0	0
55	15	5	Total Mg 5 5	0	0
55	17	2	Total Mg 2 2	0	0
55	18	3	Total Mg 3 3	0	0
55	19	3	Total Mg 3 3	0	0
55	1a	245	Total Mg 245 245	0	0
55	1b	1	Total Mg 1 1	0	0
55	1d	5	Total Mg 5 5	0	0
55	1e	1	Total Mg 1 1	0	0
55	1f	1	Total Mg 1 1	0	0
55	1g	1	Total Mg 1 1	0	0
55	1h	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1i	1	Total Mg 1 1	0	0
55	1k	1	Total Mg 1 1	0	0
55	1l	2	Total Mg 2 2	0	0
55	1n	1	Total Mg 1 1	0	0
55	1o	2	Total Mg 2 2	0	0
55	1t	1	Total Mg 1 1	0	0
55	2A	971	Total Mg 971 971	0	0
55	2B	26	Total Mg 26 26	0	0
55	2D	17	Total Mg 17 17	0	0
55	2E	6	Total Mg 6 6	0	0
55	2F	11	Total Mg 11 11	0	0
55	2G	3	Total Mg 3 3	0	0
55	2H	2	Total Mg 2 2	0	0
55	2N	3	Total Mg 3 3	0	0
55	2P	2	Total Mg 2 2	0	0
55	2Q	4	Total Mg 4 4	0	0
55	2R	3	Total Mg 3 3	0	0
55	2S	1	Total Mg 1 1	0	0
55	2T	3	Total Mg 3 3	0	0
55	2U	5	Total Mg 5 5	0	0
55	2V	5	Total Mg 5 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	2W	3	Total 3	Mg 3	0	0
55	2X	2	Total 2	Mg 2	0	0
55	2Y	1	Total 1	Mg 1	0	0
55	20	5	Total 5	Mg 5	0	0
55	21	1	Total 1	Mg 1	0	0
55	23	2	Total 2	Mg 2	0	0
55	25	4	Total 4	Mg 4	0	0
55	27	2	Total 2	Mg 2	0	0
55	28	2	Total 2	Mg 2	0	0
55	29	3	Total 3	Mg 3	0	0
55	2a	242	Total 242	Mg 242	0	0
55	2b	1	Total 1	Mg 1	0	0
55	2d	3	Total 3	Mg 3	0	0
55	2e	1	Total 1	Mg 1	0	0
55	2f	1	Total 1	Mg 1	0	0
55	2g	1	Total 1	Mg 1	0	0
55	2h	2	Total 2	Mg 2	0	0
55	2i	1	Total 1	Mg 1	0	0
55	2l	2	Total 2	Mg 2	0	0
55	2o	2	Total 2	Mg 2	0	0
55	2t	2	Total 2	Mg 2	0	0

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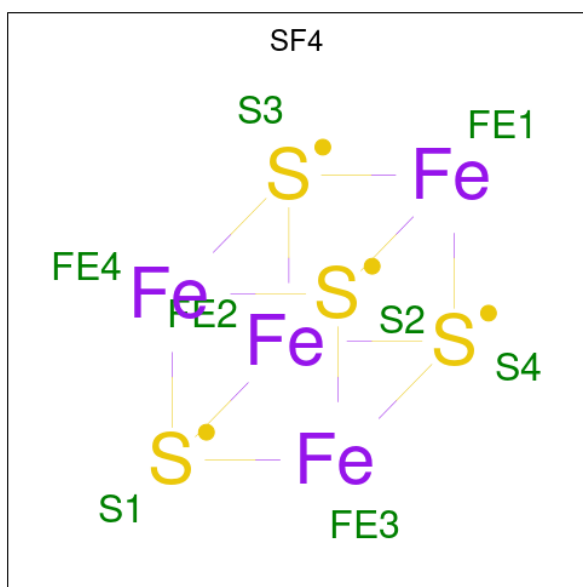
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	2z	2	Total 2	Mg 2	0	0

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1Y	1	Total 1	Zn 1	0	0
56	14	1	Total 1	Zn 1	0	0
56	15	1	Total 1	Zn 1	0	0
56	16	1	Total 1	Zn 1	0	0
56	19	1	Total 1	Zn 1	0	0
56	1n	1	Total 1	Zn 1	0	0
56	2Y	1	Total 1	Zn 1	0	0
56	24	1	Total 1	Zn 1	0	0
56	25	1	Total 1	Zn 1	0	0
56	26	1	Total 1	Zn 1	0	0
56	29	1	Total 1	Zn 1	0	0
56	2n	1	Total 1	Zn 1	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1d	1	Total	Fe S	0	0
			8	4 4		
57	2d	1	Total	Fe S	0	0
			8	4 4		

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1782	Total	O	0	0
			1782	1782		
58	1B	45	Total	O	0	0
			45	45		
58	1D	15	Total	O	0	0
			15	15		
58	1E	18	Total	O	0	0
			18	18		
58	1F	14	Total	O	0	0
			14	14		
58	1G	2	Total	O	0	0
			2	2		
58	1H	5	Total	O	0	0
			5	5		
58	1N	7	Total	O	0	0
			7	7		
58	1P	12	Total	O	0	0
			12	12		
58	1Q	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1R	6	Total 6	O 6	0	0
58	1T	5	Total 5	O 5	0	0
58	1U	7	Total 7	O 7	0	0
58	1V	3	Total 3	O 3	0	0
58	1W	1	Total 1	O 1	0	0
58	1X	6	Total 6	O 6	0	0
58	1Y	5	Total 5	O 5	0	0
58	10	6	Total 6	O 6	0	0
58	11	2	Total 2	O 2	0	0
58	13	2	Total 2	O 2	0	0
58	15	2	Total 2	O 2	0	0
58	16	2	Total 2	O 2	0	0
58	17	2	Total 2	O 2	0	0
58	18	9	Total 9	O 9	0	0
58	19	2	Total 2	O 2	0	0
58	1a	406	Total 406	O 406	0	0
58	1d	8	Total 8	O 8	0	0
58	1e	4	Total 4	O 4	0	0
58	1f	1	Total 1	O 1	0	0
58	1h	1	Total 1	O 1	0	0
58	1j	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1l	3	Total O 3 3	0	0
58	1m	3	Total O 3 3	0	0
58	1n	1	Total O 1 1	0	0
58	1o	1	Total O 1 1	0	0
58	1p	1	Total O 1 1	0	0
58	1t	1	Total O 1 1	0	0
58	1z	3	Total O 3 3	0	0
58	2A	1771	Total O 1771 1771	0	0
58	2B	46	Total O 46 46	0	0
58	2D	14	Total O 14 14	0	0
58	2E	20	Total O 20 20	0	0
58	2F	12	Total O 12 12	0	0
58	2G	2	Total O 2 2	0	0
58	2H	4	Total O 4 4	0	0
58	2N	7	Total O 7 7	0	0
58	2P	11	Total O 11 11	0	0
58	2Q	7	Total O 7 7	0	0
58	2R	6	Total O 6 6	0	0
58	2T	5	Total O 5 5	0	0
58	2U	8	Total O 8 8	0	0
58	2V	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2W	2	Total 2	O 2	0	0
58	2X	7	Total 7	O 7	0	0
58	2Y	5	Total 5	O 5	0	0
58	20	8	Total 8	O 8	0	0
58	21	2	Total 2	O 2	0	0
58	23	2	Total 2	O 2	0	0
58	25	4	Total 4	O 4	0	0
58	26	2	Total 2	O 2	0	0
58	27	2	Total 2	O 2	0	0
58	28	11	Total 11	O 11	0	0
58	29	2	Total 2	O 2	0	0
58	2a	404	Total 404	O 404	0	0
58	2d	8	Total 8	O 8	0	0
58	2e	6	Total 6	O 6	0	0
58	2f	1	Total 1	O 1	0	0
58	2h	1	Total 1	O 1	0	0
58	2j	1	Total 1	O 1	0	0
58	2l	3	Total 3	O 3	0	0
58	2m	2	Total 2	O 2	0	0
58	2n	1	Total 1	O 1	0	0
58	2o	3	Total 3	O 3	0	0

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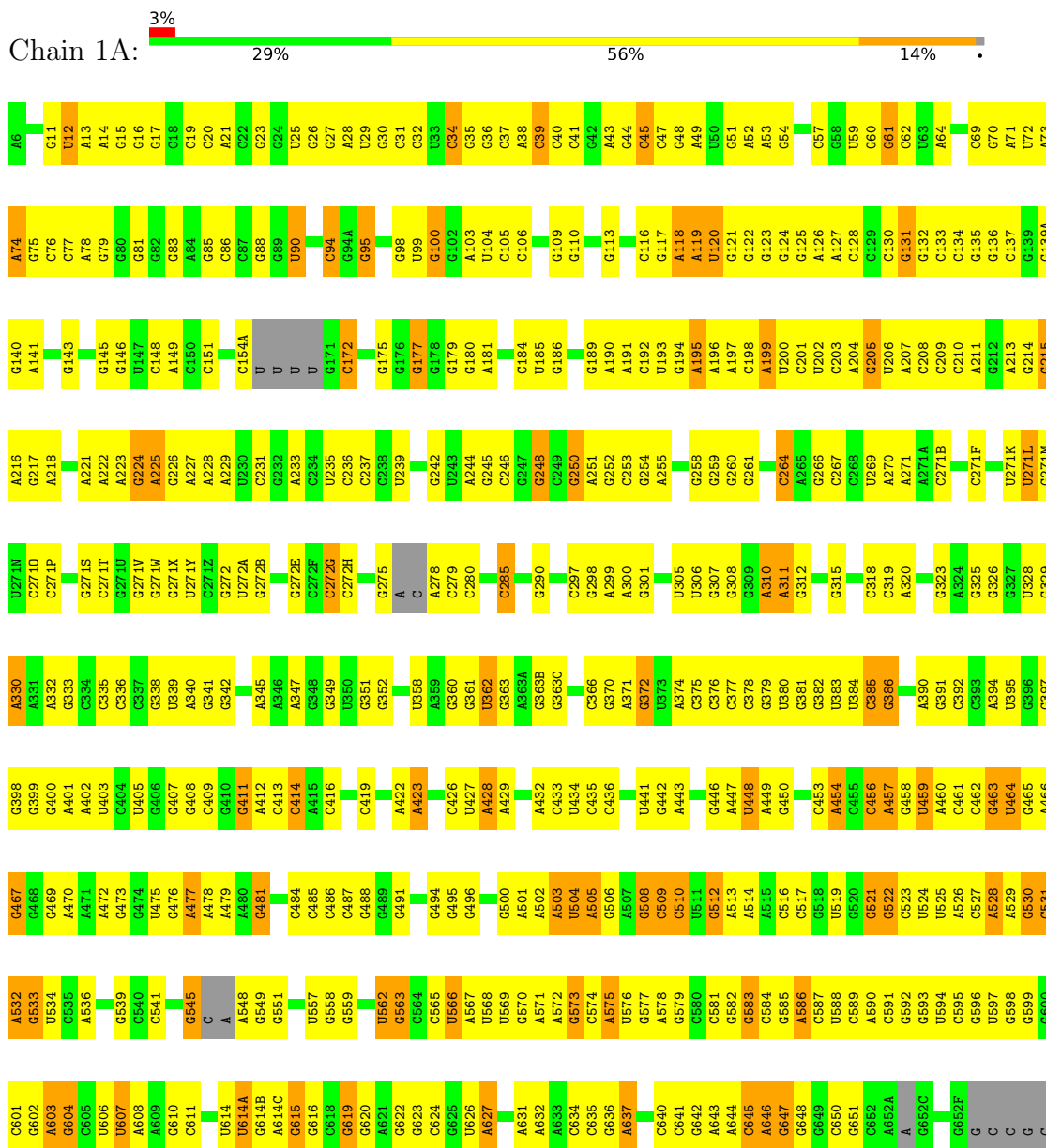
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
58	2p	1	Total O 1 1	0	0
58	2z	4	Total O 4 4	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

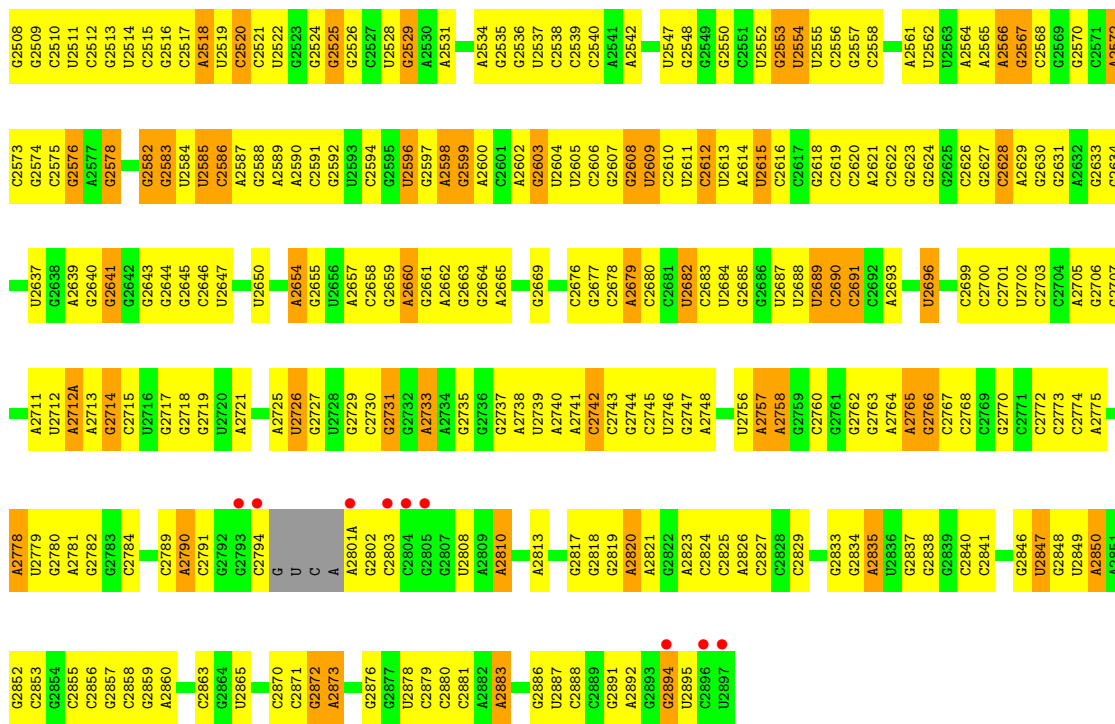
- Molecule 1: 23S ribosomal RNA



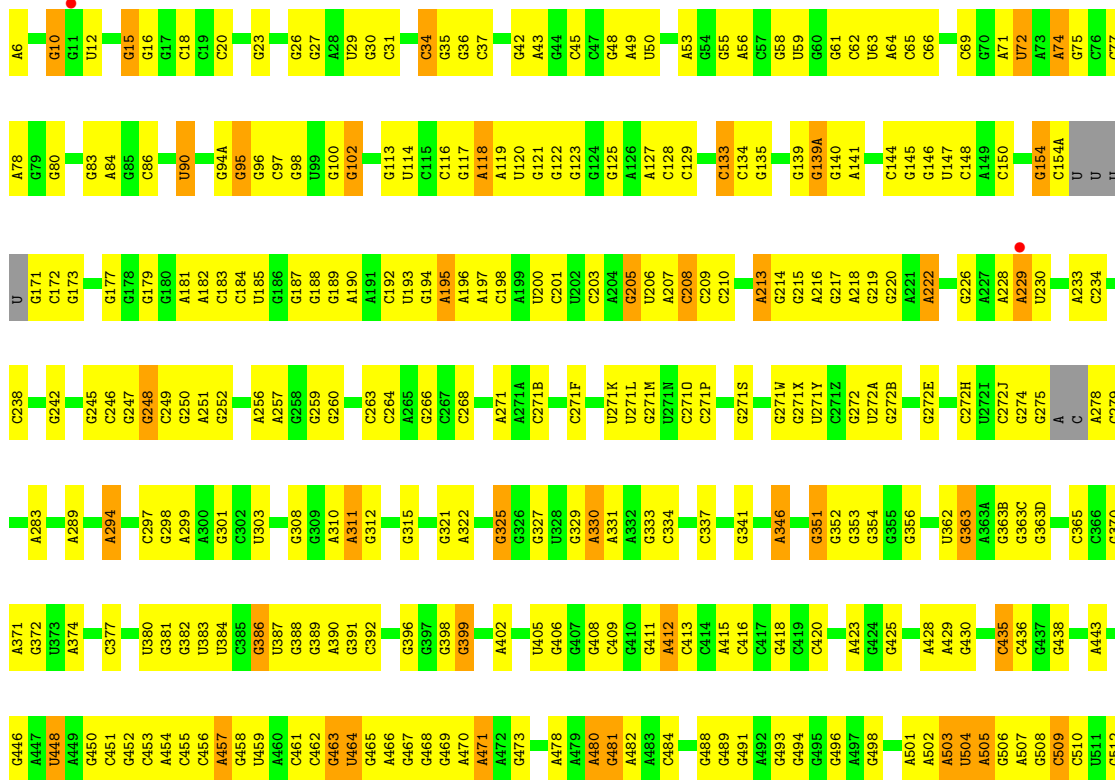
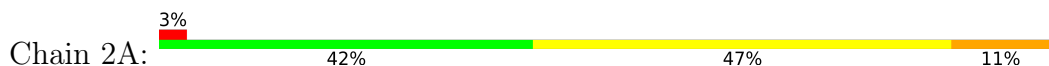
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U1340	U1341	U1342	U1343	U1344	U1345	U1346	U1347	U1348	U1349	U1350	U1351	U1352	U1353	U1354	U1355	U1356	U1357	U1358	U1359	U1360	U1361	U1362	U1363	U1364	U1365	U1366	U1367	U1368	U1369	U1370	U1371	U1372	U1373	U1374	U1375	U1376	U1377	U1378	U1379	U1380	U1381	U1382	U1383	U1384	U1385	U1386	U1387	U1390	U1391	U1392	U1393	U1394	U1395	U1396	U1397	U1398	U1399	U1400	U1401	U1402	U1403	U1404	U1405	U1406	U1407	U1408	U1409	U1410	U1411	U1412	U1413	U1414	U1415	U1416	U1417	U1418	U1419	U1420	U1421	U1422	U1423	U1424	U1425	U1426	U1427	U1428	U1429	U1430	U1431	U1432	U1433	U1434	U1435	U1436	U1437	U1438	U1439	U1440	U1441	U1442	U1443	U1444	U1445	U1446	U1447	U1448	U1449	U1450	U1452	U1453	U1454	U1455	U1456	U1459	U1460	U1466	U1467	U1468	U1469																	
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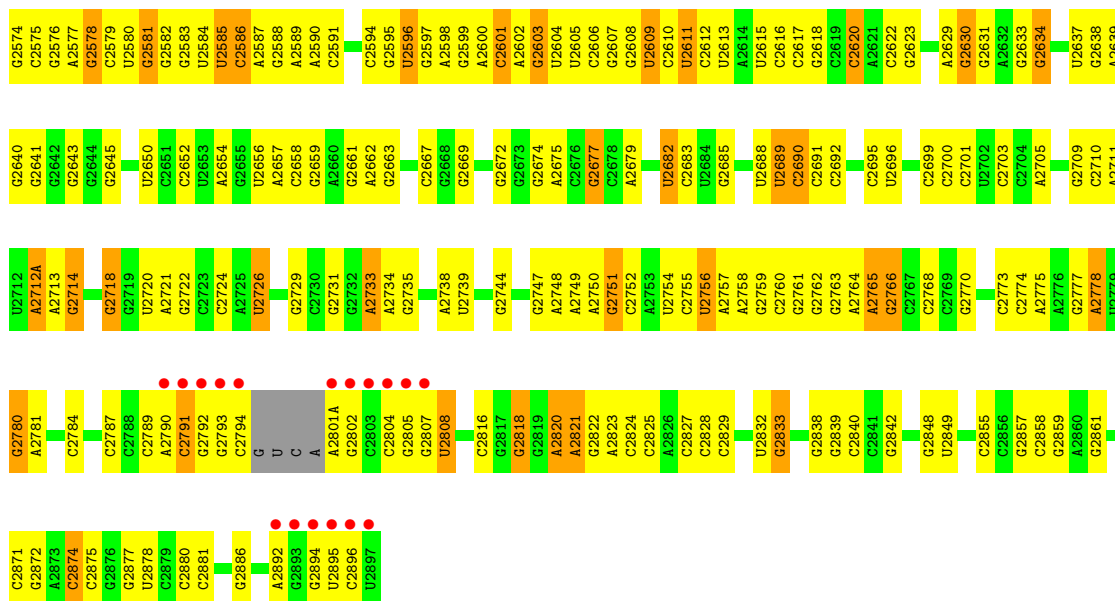


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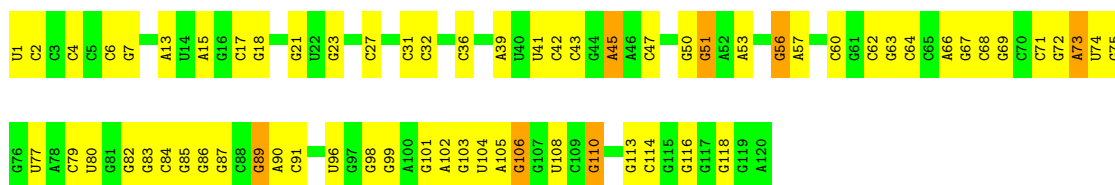




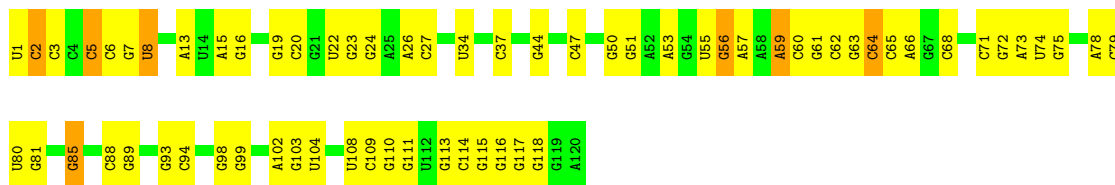




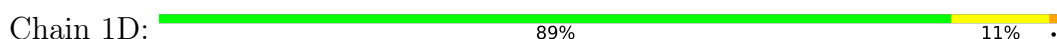
• Molecule 2: 5S ribosomal RNA



• Molecule 2: 5S ribosomal RNA



• Molecule 3: 50S ribosomal protein L2

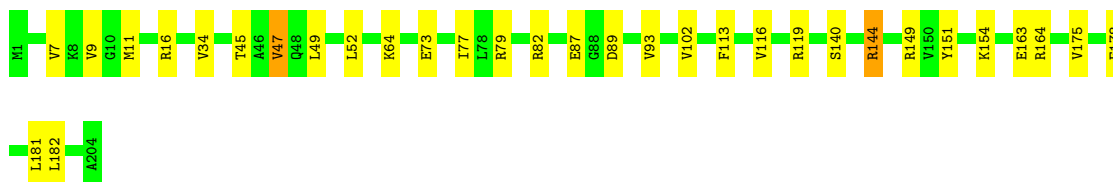
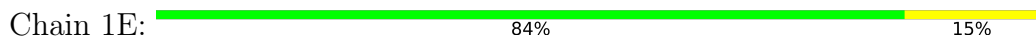


• Molecule 3: 50S ribosomal protein L2

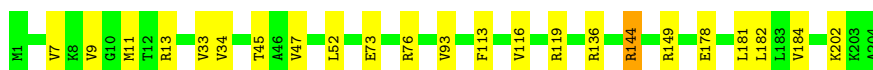
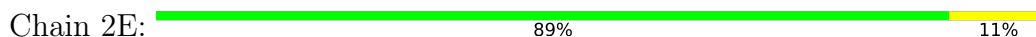




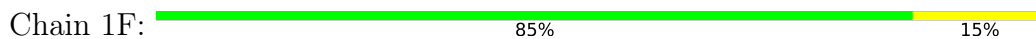
- Molecule 4: 50S ribosomal protein L3



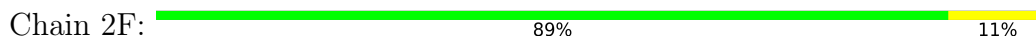
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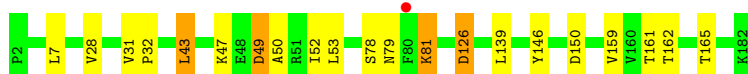
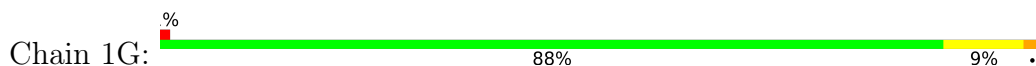
- Molecule 5: 50S ribosomal protein L4



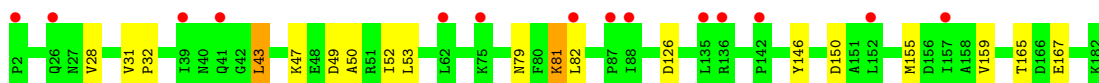
- Molecule 5: 50S ribosomal protein L4



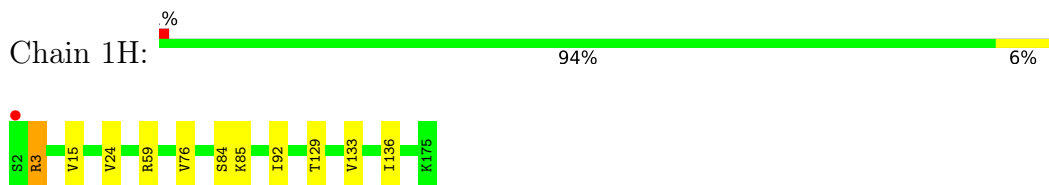
- Molecule 6: 50S ribosomal protein L5



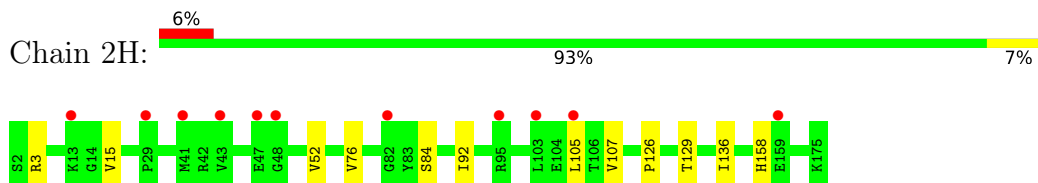
- Molecule 6: 50S ribosomal protein L5



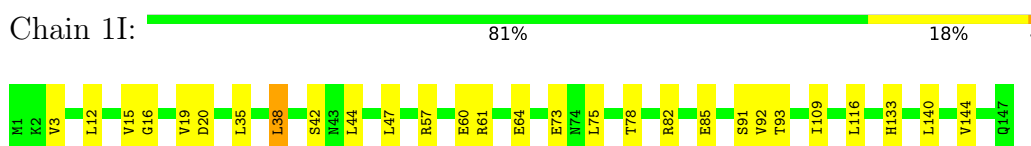
- Molecule 7: 50S ribosomal protein L6



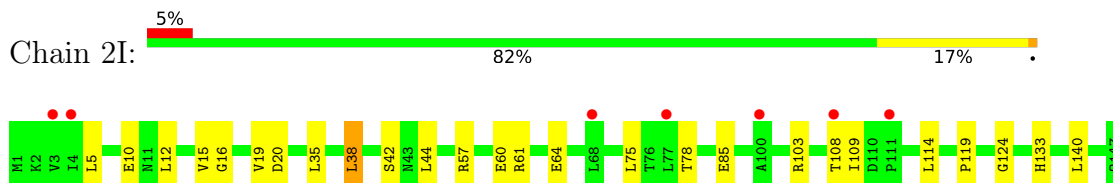
- Molecule 7: 50S ribosomal protein L6



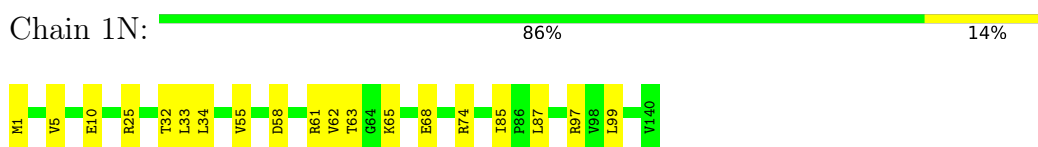
- Molecule 8: 50S ribosomal protein L9



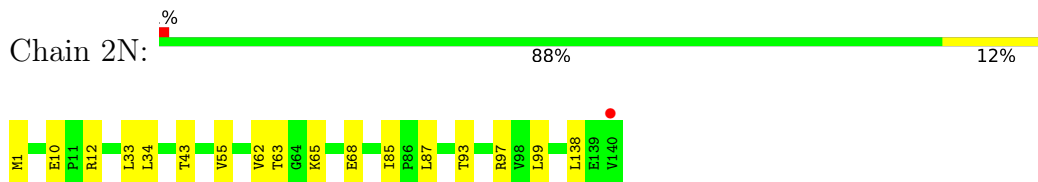
- Molecule 8: 50S ribosomal protein L9



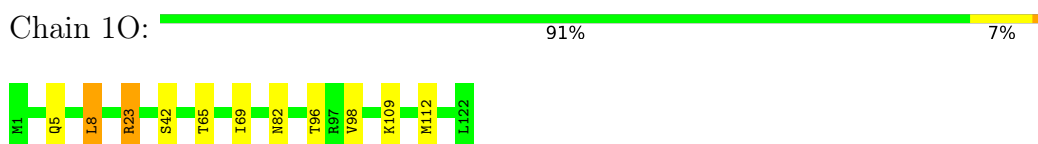
- Molecule 9: 50S ribosomal protein L13



- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14



- Molecule 10: 50S ribosomal protein L14

Chain 2O:  92% 7%

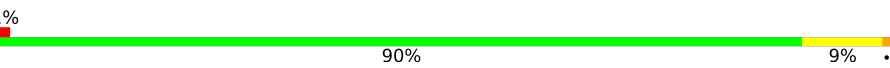


- Molecule 11: 50S ribosomal protein L15

Chain 1P:  91% 8%



- Molecule 11: 50S ribosomal protein L15

Chain 2P:  90% 9%



- Molecule 12: 50S ribosomal protein L16

Chain 1Q:  90% 10%




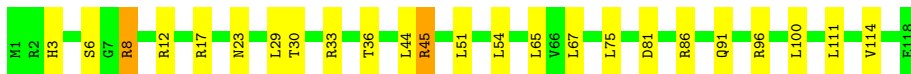
- Molecule 12: 50S ribosomal protein L16

Chain 2Q:  90% 9%




- Molecule 13: 50S ribosomal protein L17

Chain 1R:  80% 19%



- Molecule 13: 50S ribosomal protein L17

Chain 2R:  87% 12%



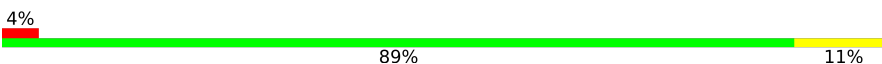


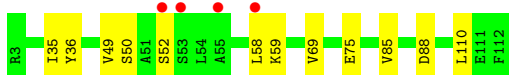
- Molecule 14: 50S ribosomal protein L18

Chain 1S:  86% 14%



- Molecule 14: 50S ribosomal protein L18

Chain 2S:  4% 89% 11%



- Molecule 15: 50S ribosomal protein L19

Chain 1T:  89% 10%




- Molecule 15: 50S ribosomal protein L19

Chain 2T:  92% 8%



- Molecule 16: 50S ribosomal protein L20

Chain 1U:  84% 16%




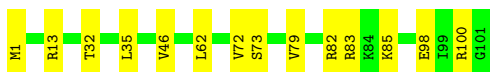
- Molecule 16: 50S ribosomal protein L20

Chain 2U:  89% 11%



- Molecule 17: 50S ribosomal protein L21

Chain 1V:  86% 14%



- Molecule 17: 50S ribosomal protein L21

Chain 2V:  92% 8%




- Molecule 18: 50S ribosomal protein L22

Chain 1W:  88% 12%



- Molecule 18: 50S ribosomal protein L22

Chain 2W:  86% 14%



- Molecule 19: 50S ribosomal protein L23

Chain 1X:  95% 5%




- Molecule 19: 50S ribosomal protein L23

Chain 2X:  94% 6%




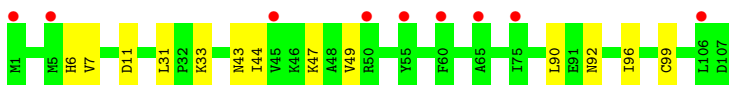
- Molecule 20: 50S ribosomal protein L24

Chain 1Y:  87% 13%




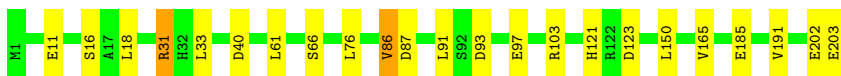
- Molecule 20: 50S ribosomal protein L24

Chain 2Y:  88% 12%

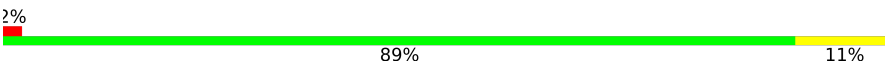


- Molecule 21: 50S ribosomal protein L25

Chain 1Z:  89% 10%



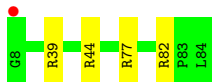
- Molecule 21: 50S ribosomal protein L25

Chain 2Z:  89% 11% 2%



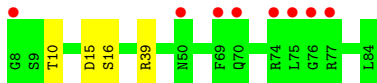
- Molecule 22: 50S ribosomal protein L27

Chain 10:  95% 5% 1%



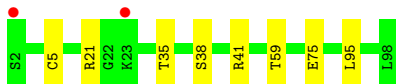
- Molecule 22: 50S ribosomal protein L27

Chain 20:  95% 5% 10%



- Molecule 23: 50S ribosomal protein L28

Chain 11:  92% 8% 2%



- Molecule 23: 50S ribosomal protein L28

Chain 21:  95% 1% 1%

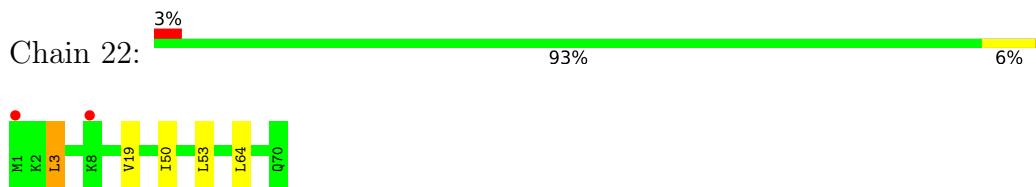


- Molecule 24: 50S ribosomal protein L29

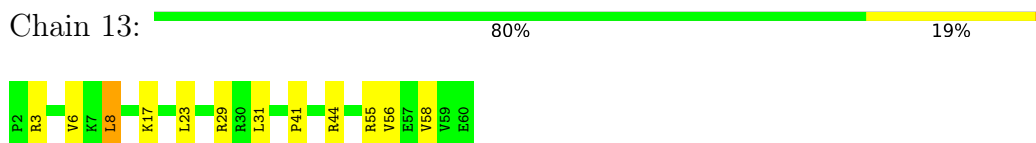
Chain 12:  90% 10%



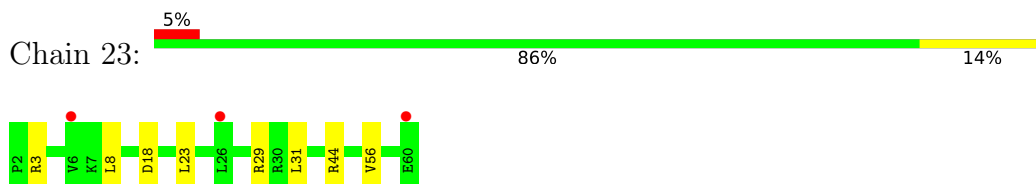
- Molecule 24: 50S ribosomal protein L29



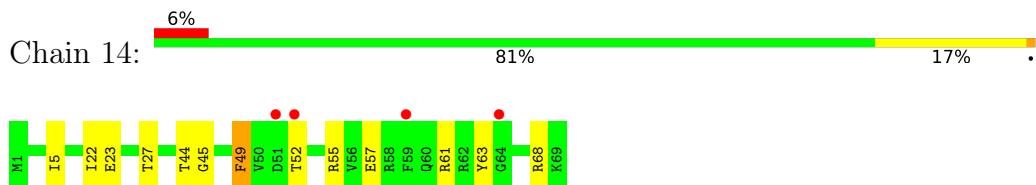
- Molecule 25: 50S ribosomal protein L30



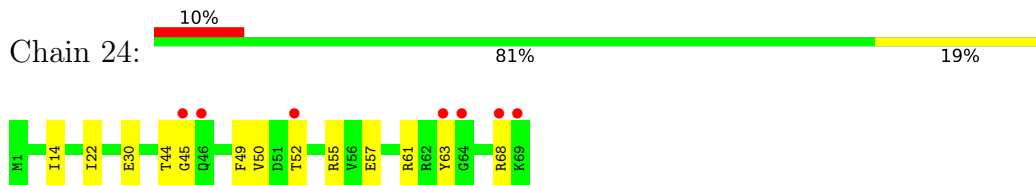
- Molecule 25: 50S ribosomal protein L30



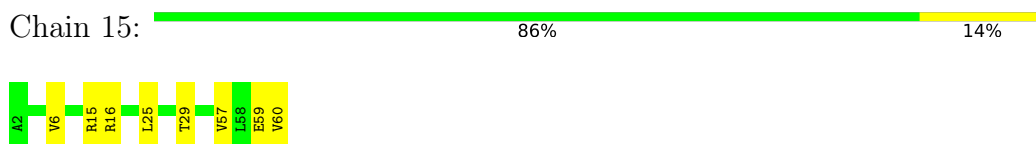
- Molecule 26: 50S ribosomal protein L31



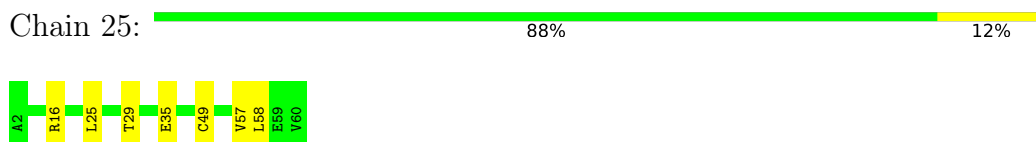
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33

Chain 16:  85% 15%




- Molecule 28: 50S ribosomal protein L33

Chain 26:  91% 9%




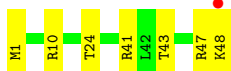
- Molecule 29: 50S ribosomal protein L34

Chain 17:  83% 15% 2%




- Molecule 29: 50S ribosomal protein L34

Chain 27:  85% 15% 2%



- Molecule 30: 50S ribosomal protein L35

Chain 18:  89% 11%




- Molecule 30: 50S ribosomal protein L35

Chain 28:  92% 8%

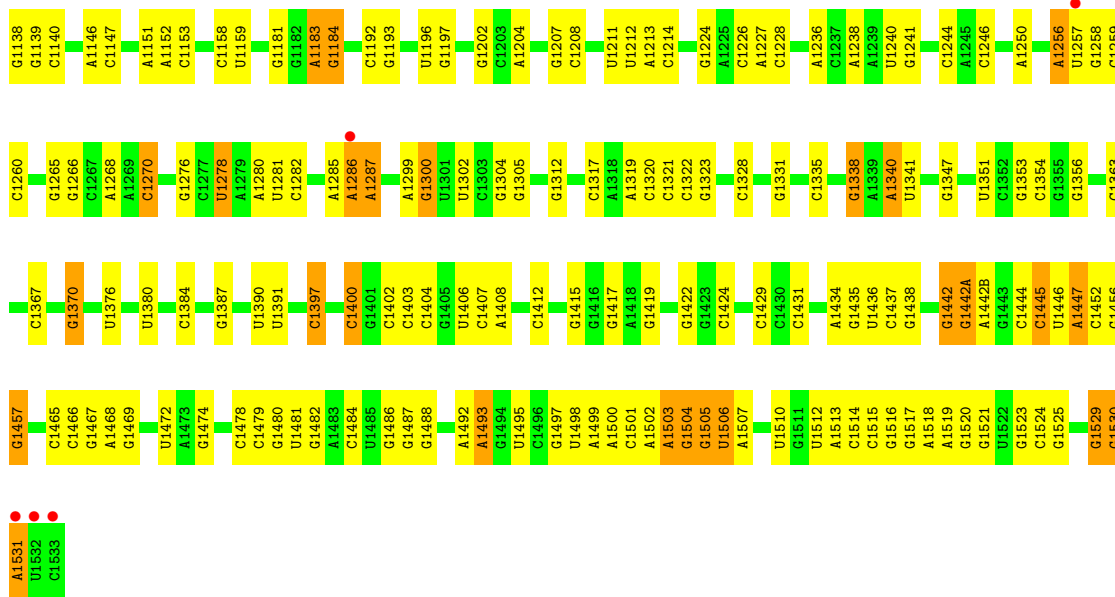


- Molecule 31: 50S ribosomal protein L36

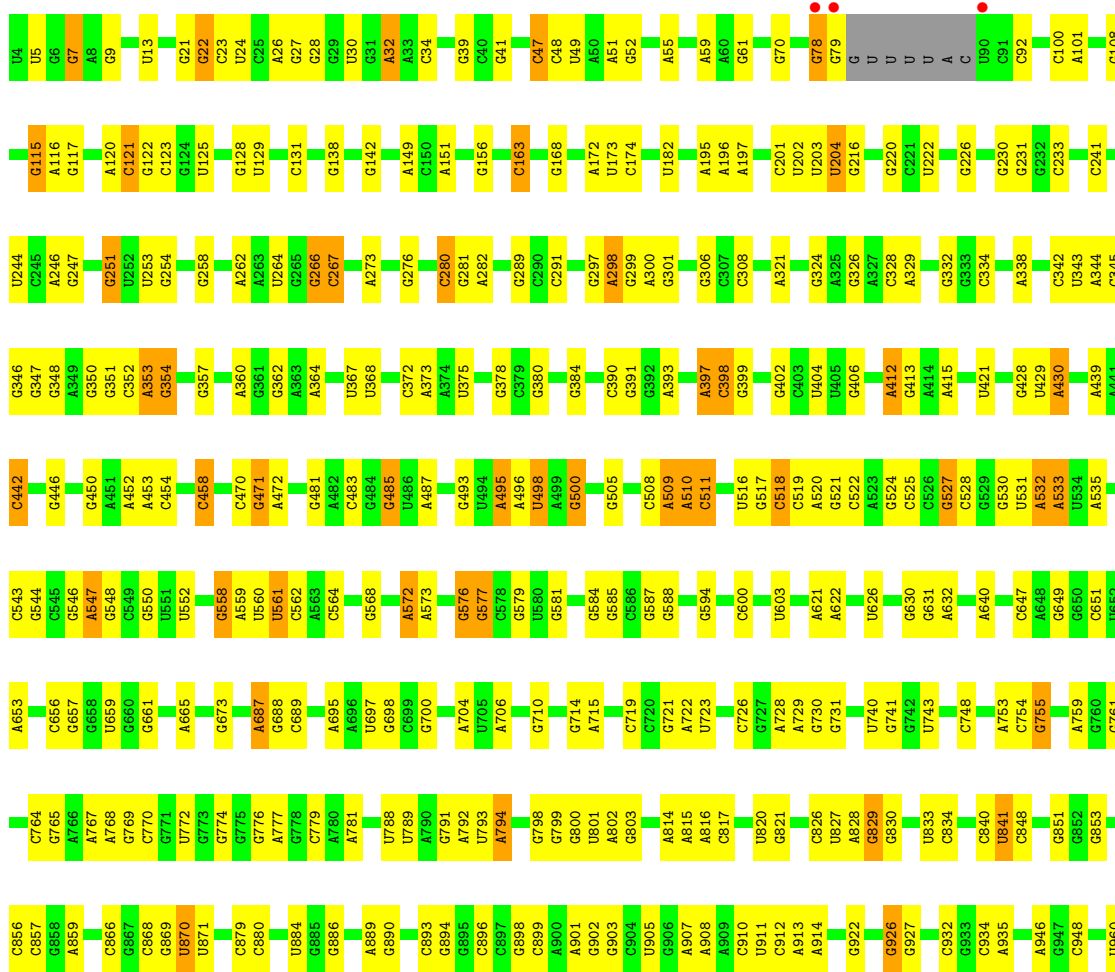
Chain 19:  86% 14%

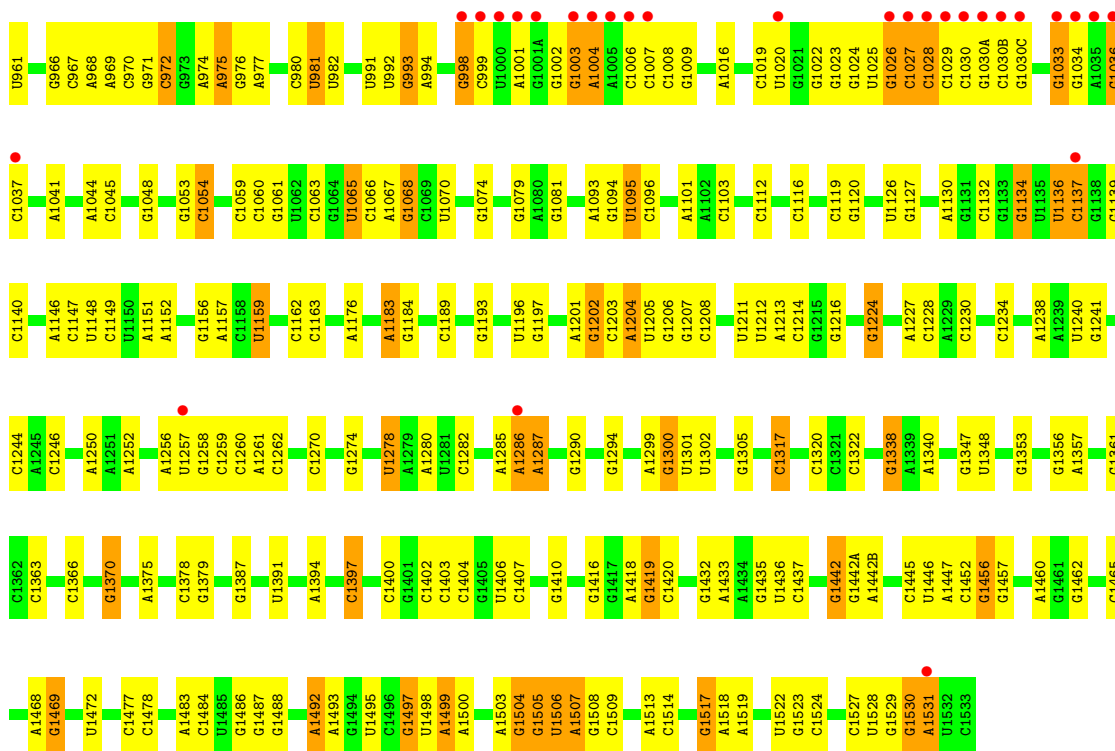




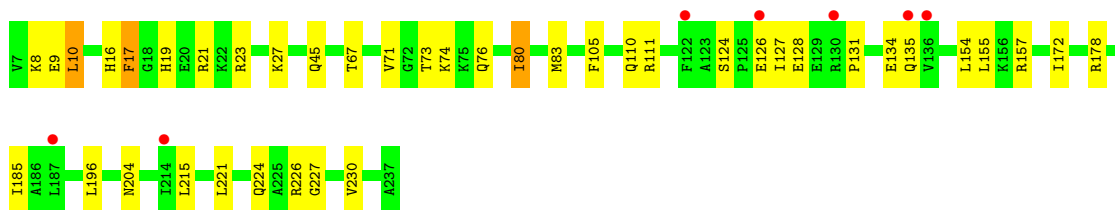
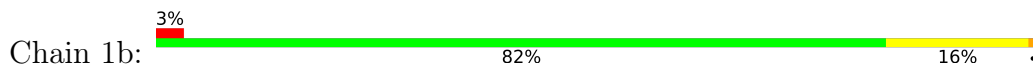


• Molecule 32: 16 ribosomal RNA

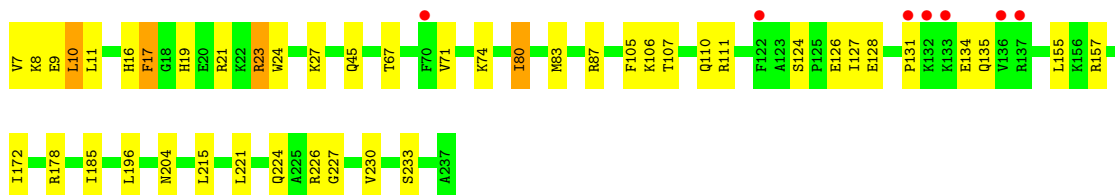
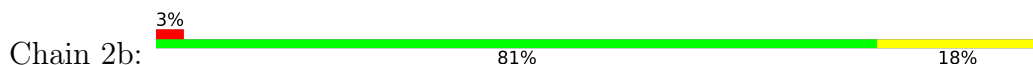




• Molecule 33: 30S ribosomal protein S2



• Molecule 33: 30S ribosomal protein S2

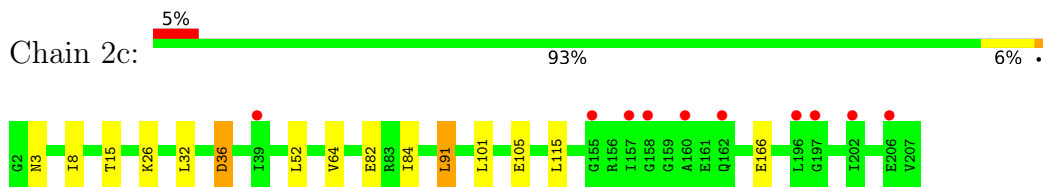


• Molecule 34: 30S ribosomal protein S3

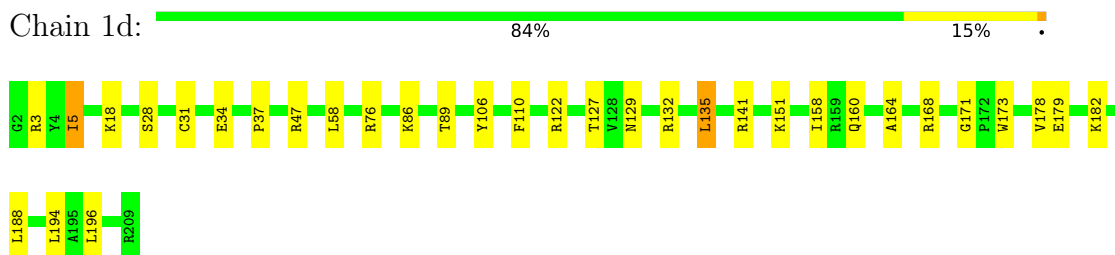




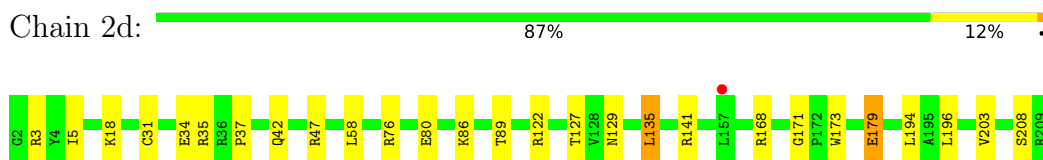
- Molecule 34: 30S ribosomal protein S3



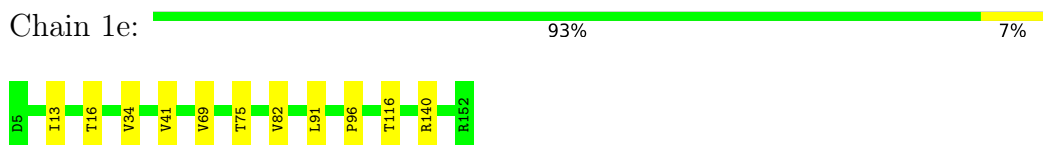
- Molecule 35: 30S ribosomal protein S4



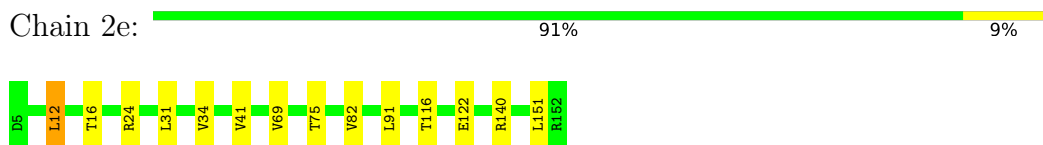
- Molecule 35: 30S ribosomal protein S4



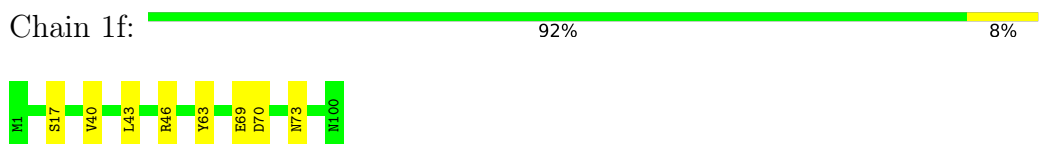
- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6

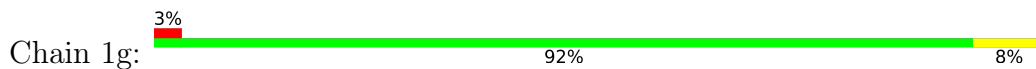


- Molecule 37: 30S ribosomal protein S6

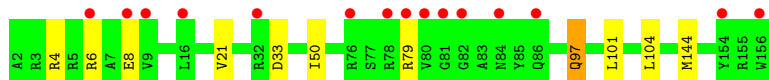




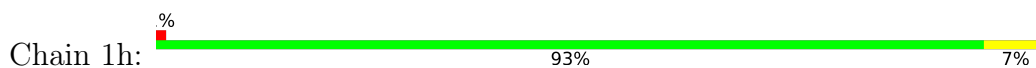
- Molecule 38: 30S ribosomal protein S7



- Molecule 38: 30S ribosomal protein S7



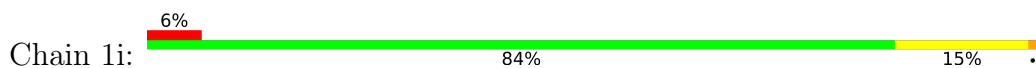
- Molecule 39: 30S ribosomal protein S8



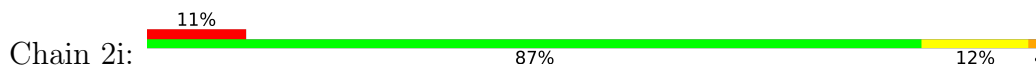
- Molecule 39: 30S ribosomal protein S8



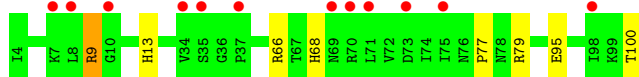
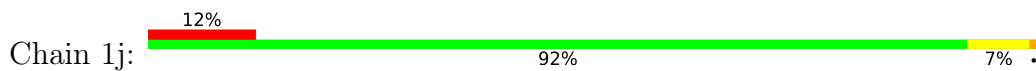
- Molecule 40: 30S ribosomal protein S9



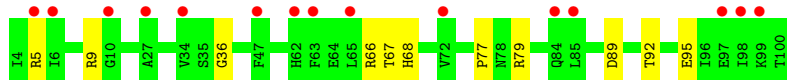
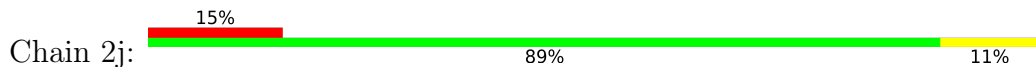
- Molecule 40: 30S ribosomal protein S9



- Molecule 41: 30S ribosomal protein S10



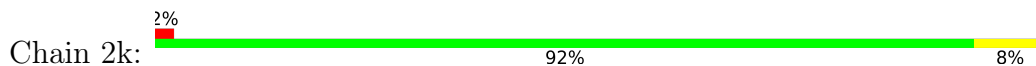
- Molecule 41: 30S ribosomal protein S10



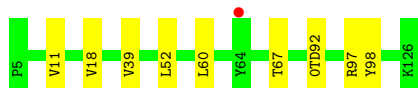
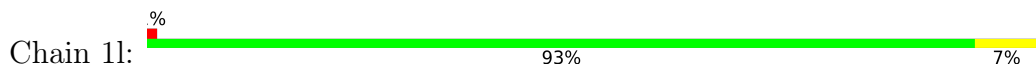
- Molecule 42: 30S ribosomal protein S11



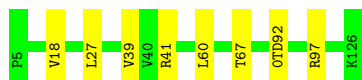
- Molecule 42: 30S ribosomal protein S11



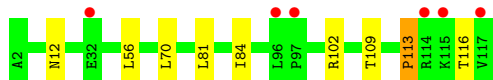
- Molecule 43: 30S ribosomal protein S12



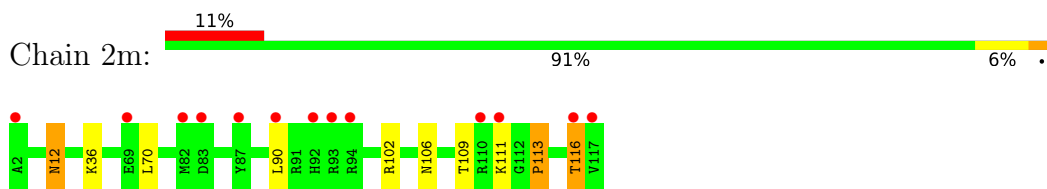
- Molecule 43: 30S ribosomal protein S12



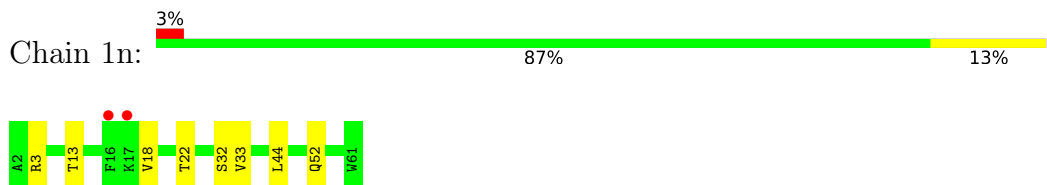
- Molecule 44: 30S ribosomal protein S13



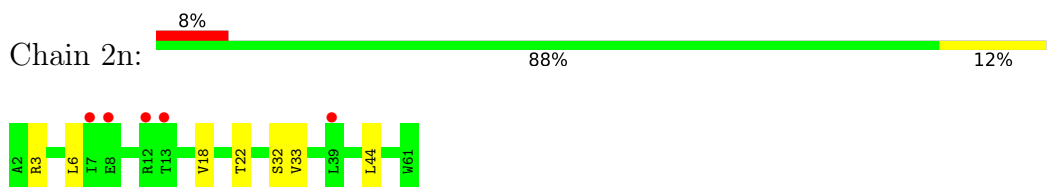
- Molecule 44: 30S ribosomal protein S13



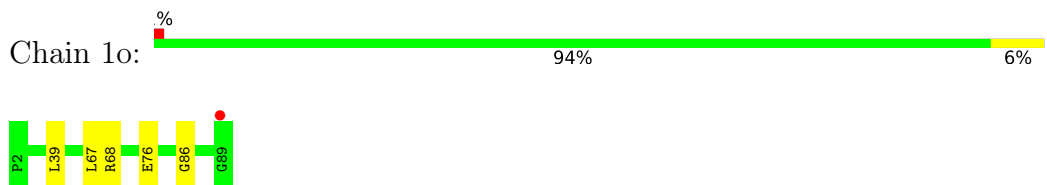
- Molecule 45: 30S ribosomal protein S14 type Z



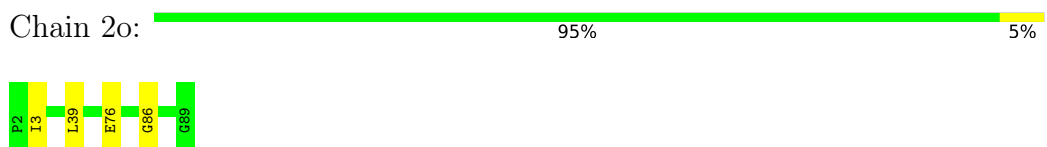
- Molecule 45: 30S ribosomal protein S14 type Z



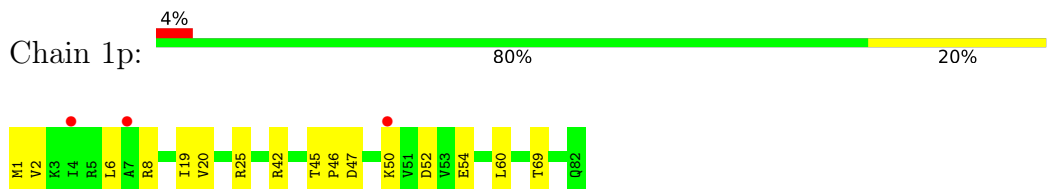
- Molecule 46: 30S ribosomal protein S15



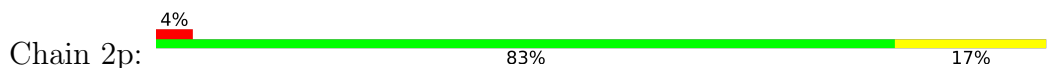
- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16

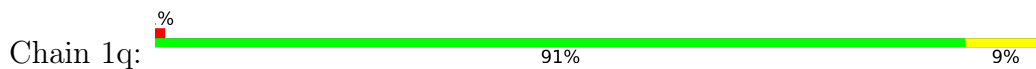


- Molecule 47: 30S ribosomal protein S16





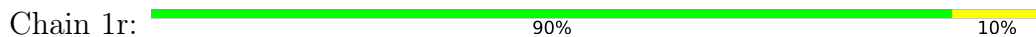
- Molecule 48: 30S ribosomal protein S17



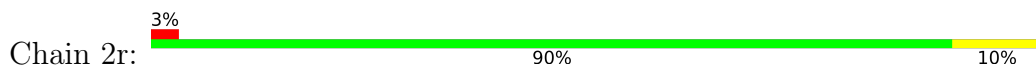
- Molecule 48: 30S ribosomal protein S17



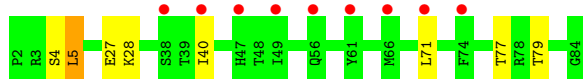
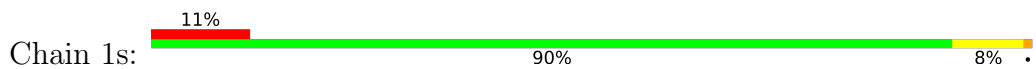
- Molecule 49: 30S ribosomal protein S18



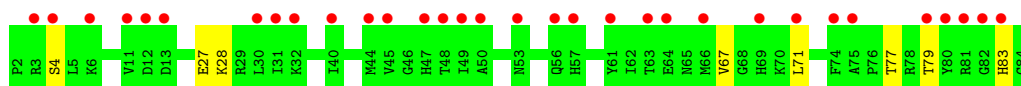
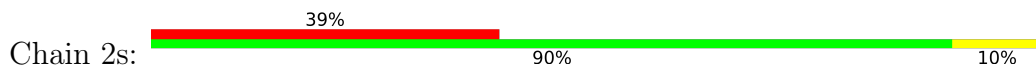
- Molecule 49: 30S ribosomal protein S18



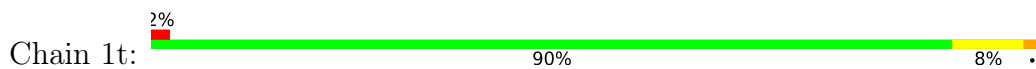
- Molecule 50: 30S ribosomal protein S19



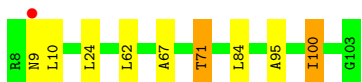
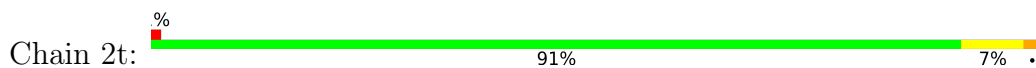
- Molecule 50: 30S ribosomal protein S19



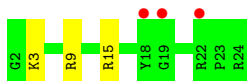
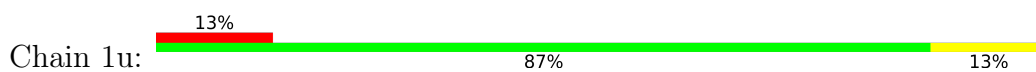
- Molecule 51: 30S ribosomal protein S20



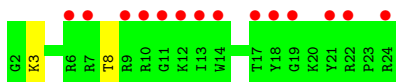
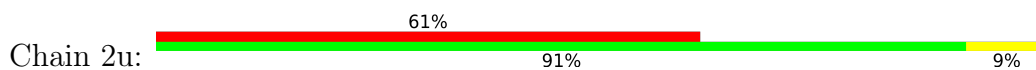
- Molecule 51: 30S ribosomal protein S20



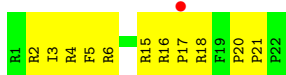
- Molecule 52: 30S ribosomal protein Thx



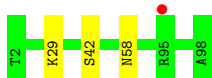
- Molecule 52: 30S ribosomal protein Thx



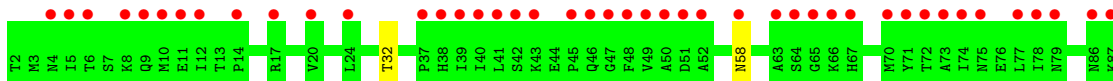
- Molecule 53: Tur1A peptide

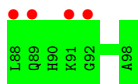


- Molecule 54: Ribosome-associated inhibitor A



- Molecule 54: Ribosome-associated inhibitor A





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.68Å 449.25Å 621.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.76 – 3.20 49.76 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.76-3.20) 98.6 (49.76-3.20)	Depositor EDS
$R_{merge}$	0.39	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, $R_{free}$	0.190 , 0.252 0.191 , 0.252	Depositor DCC
$R_{free}$ test set	47082 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.9	Xtrriage
Anisotropy	0.208	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 67.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	294294	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, 2MG, 5MC, UR3, 2MU, OMG, 0TD, 2MA, SF4, MG, PSU, M2G, 7MG, 5MU, ZN, 4OC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	1A	1.48	500/69032 (0.7%)	2.18	4548/107750 (4.2%)
1	2A	1.16	115/69032 (0.2%)	1.90	2782/107750 (2.6%)
2	1B	1.18	2/2879 (0.1%)	1.99	140/4490 (3.1%)
2	2B	1.12	4/2879 (0.1%)	1.83	98/4490 (2.2%)
3	1D	0.98	0/2181	1.14	8/2940 (0.3%)
3	2D	0.83	0/2181	1.05	7/2940 (0.2%)
4	1E	0.98	2/1592 (0.1%)	1.13	10/2149 (0.5%)
4	2E	0.82	0/1592	1.04	5/2149 (0.2%)
5	1F	0.96	0/1619	1.00	1/2193 (0.0%)
5	2F	0.71	0/1619	0.88	1/2193 (0.0%)
6	1G	0.61	0/1451	0.86	0/1961
6	2G	0.66	1/1451 (0.1%)	0.86	1/1961 (0.1%)
7	1H	0.84	0/1356	0.94	1/1834 (0.1%)
7	2H	0.72	0/1356	0.86	0/1834
8	1I	0.66	0/1109	0.90	1/1512 (0.1%)
8	2I	0.71	1/1109 (0.1%)	1.00	3/1512 (0.2%)
9	1N	0.93	0/1148	1.03	3/1547 (0.2%)
9	2N	0.71	0/1148	0.92	0/1547
10	1O	0.99	0/943	1.03	3/1269 (0.2%)
10	2O	0.84	0/943	1.00	1/1269 (0.1%)
11	1P	0.90	0/1152	1.07	2/1533 (0.1%)
11	2P	0.76	1/1152 (0.1%)	0.96	1/1533 (0.1%)
12	1Q	0.90	1/1143 (0.1%)	0.98	2/1527 (0.1%)
12	2Q	0.76	0/1143	0.96	2/1527 (0.1%)
13	1R	0.93	0/982	1.15	7/1312 (0.5%)
13	2R	0.75	0/982	1.00	2/1312 (0.2%)
14	1S	0.78	0/887	0.96	1/1180 (0.1%)
14	2S	0.73	0/887	0.97	1/1180 (0.1%)
15	1T	0.93	0/1105	1.06	2/1477 (0.1%)
15	2T	0.78	0/1105	0.99	2/1477 (0.1%)
16	1U	1.07	1/977 (0.1%)	1.09	4/1301 (0.3%)
16	2U	0.76	0/977	0.93	1/1301 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	1V	0.96	0/786	1.09	3/1053 (0.3%)
17	2V	0.75	0/786	0.92	0/1053
18	1W	1.05	0/897	1.11	3/1205 (0.2%)
18	2W	0.89	0/897	1.09	4/1205 (0.3%)
19	1X	1.01	0/764	1.00	0/1025
19	2X	0.85	0/764	0.98	0/1025
20	1Y	0.94	1/823 (0.1%)	1.01	1/1099 (0.1%)
20	2Y	0.77	0/823	1.00	2/1099 (0.2%)
21	1Z	0.74	0/1620	0.88	2/2200 (0.1%)
21	2Z	0.65	0/1620	0.90	1/2200 (0.0%)
22	10	0.93	0/616	1.08	3/821 (0.4%)
22	20	0.78	0/616	1.01	1/821 (0.1%)
23	11	0.99	0/761	0.99	1/1013 (0.1%)
23	21	0.82	0/761	0.96	1/1013 (0.1%)
24	12	0.82	0/590	0.96	1/781 (0.1%)
24	22	0.75	0/590	0.91	1/781 (0.1%)
25	13	0.98	0/474	1.07	3/635 (0.5%)
25	23	0.70	0/474	0.94	1/635 (0.2%)
26	14	0.64	0/559	0.86	0/754
26	24	0.70	0/559	0.86	0/754
27	15	1.02	1/473 (0.2%)	1.02	1/639 (0.2%)
27	25	0.82	1/473 (0.2%)	0.98	1/639 (0.2%)
28	16	0.87	0/460	0.93	0/613
28	26	0.72	0/460	0.92	0/613
29	17	1.06	0/426	1.01	2/561 (0.4%)
29	27	0.85	0/426	1.03	0/561
30	18	1.02	1/525 (0.2%)	0.99	1/691 (0.1%)
30	28	0.78	0/525	0.91	0/691
31	19	0.97	1/310 (0.3%)	0.98	0/407
31	29	0.74	0/310	0.95	0/407
32	1a	0.99	28/35795 (0.1%)	1.67	838/55864 (1.5%)
32	2a	0.96	18/35795 (0.1%)	1.63	747/55864 (1.3%)
33	1b	0.62	0/1876	0.86	0/2533
33	2b	0.61	0/1876	0.88	1/2533 (0.0%)
34	1c	0.53	0/1582	0.76	0/2137
34	2c	0.59	0/1582	0.81	2/2137 (0.1%)
35	1d	0.61	0/1695	0.81	1/2274 (0.0%)
35	2d	0.60	0/1695	0.88	1/2274 (0.0%)
36	1e	0.62	0/1149	0.86	0/1548
36	2e	0.64	1/1149 (0.1%)	0.87	2/1548 (0.1%)
37	1f	0.67	0/827	0.86	0/1120
37	2f	0.63	0/827	0.88	0/1120
38	1g	0.57	0/1254	0.76	0/1683

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	2g	0.56	0/1254	0.80	1/1683 (0.1%)
39	1h	0.64	0/1118	0.83	0/1506
39	2h	0.57	0/1118	0.84	0/1506
40	1i	0.55	0/1005	0.79	0/1351
40	2i	0.58	0/1005	0.79	0/1351
41	1j	0.56	0/732	0.82	1/993 (0.1%)
41	2j	0.56	0/732	0.81	0/993
42	1k	0.65	0/849	0.81	0/1150
42	2k	0.67	1/849 (0.1%)	0.83	1/1150 (0.1%)
43	1l	0.68	0/937	0.87	0/1260
43	2l	0.67	0/937	0.87	0/1260
44	1m	0.53	0/924	0.78	0/1242
44	2m	0.64	0/924	0.84	1/1242 (0.1%)
45	1n	0.56	0/501	0.81	0/664
45	2n	0.60	0/501	0.75	0/664
46	1o	0.61	0/739	0.86	1/985 (0.1%)
46	2o	0.59	0/739	0.88	0/985
47	1p	0.56	0/697	0.85	0/939
47	2p	0.65	0/697	0.83	0/939
48	1q	0.68	0/836	0.90	0/1117
48	2q	0.66	0/836	0.87	0/1117
49	1r	0.63	0/560	0.87	0/746
49	2r	0.70	0/560	0.86	0/746
50	1s	0.53	0/663	0.80	1/895 (0.1%)
50	2s	0.65	0/663	0.76	0/895
51	1t	0.61	0/734	0.87	0/969
51	2t	0.56	0/734	0.82	0/969
52	1u	0.51	0/203	0.83	0/266
52	2u	0.56	0/203	0.83	0/266
53	1y	0.94	0/177	1.15	0/245
54	1z	0.64	0/776	0.84	0/1048
54	2z	0.71	0/776	0.82	0/1048
All	All	1.10	681/310361 (0.2%)	1.71	9271/463769 (2.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	1E	0	1
4	2E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	1S	0	1
14	2S	0	1
15	1T	0	1
15	2T	0	1
19	1X	0	1
19	2X	0	1
33	2b	0	1
44	1m	0	1
44	2m	0	1
53	1y	0	1
All	All	0	12

All (681) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	807	U	C2-N3	9.44	1.44	1.37
1	2A	2573	C	N3-C4	9.04	1.40	1.33
1	1A	783	A	C6-N1	-8.93	1.29	1.35
1	2A	687	C	N1-C6	-8.56	1.32	1.37
1	1A	2032	G	N7-C5	-8.51	1.34	1.39
1	1A	2058	A	N3-C4	-8.50	1.29	1.34
1	1A	2057	A	N9-C4	-8.48	1.32	1.37
1	1A	2690	C	N1-C6	-8.40	1.32	1.37
1	2A	675	A	N9-C4	-8.40	1.32	1.37
1	2A	2478	A	N9-C4	-8.36	1.32	1.37
1	1A	1046	A	N9-C4	8.21	1.42	1.37
1	1A	2392	A	N3-C4	-8.20	1.29	1.34
1	1A	1189	A	N9-C4	-8.08	1.33	1.37
1	1A	197	A	N3-C4	-8.04	1.30	1.34
1	1A	2033	A	N3-C4	-8.02	1.30	1.34
1	1A	332	A	N9-C4	-7.98	1.33	1.37
1	1A	2610	C	N1-C6	-7.98	1.32	1.37
1	1A	1127	A	N9-C4	-7.96	1.33	1.37
1	1A	2249	U	C2-N3	-7.95	1.32	1.37
1	1A	2589	A	N9-C4	-7.89	1.33	1.37
1	1A	1367	A	N9-C4	-7.84	1.33	1.37
1	1A	1021	A	N9-C4	-7.83	1.33	1.37
1	1A	2021	C	N1-C6	-7.81	1.32	1.37
1	1A	1253	A	N7-C5	-7.81	1.34	1.39
1	1A	2430	A	N3-C4	-7.79	1.30	1.34
1	1A	2013	A	N7-C5	-7.76	1.34	1.39
1	1A	591	C	N3-C4	-7.76	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2542	A	N3-C4	-7.70	1.30	1.34
1	1A	2641	G	N7-C5	-7.69	1.34	1.39
1	1A	1660	C	N3-C4	-7.68	1.28	1.33
32	2a	1492	A	N9-C4	7.63	1.42	1.37
1	1A	2758	A	N9-C4	-7.62	1.33	1.37
1	1A	2258	C	N1-C6	-7.57	1.32	1.37
1	1A	198	C	N1-C6	-7.55	1.32	1.37
1	2A	229	A	N9-C4	7.53	1.42	1.37
1	1A	599	G	N9-C8	-7.48	1.32	1.37
1	1A	911	A	C5-C6	-7.48	1.34	1.41
1	1A	2060	A	C6-N1	-7.46	1.30	1.35
1	1A	2442	C	N1-C6	-7.43	1.32	1.37
1	1A	472	A	N3-C4	-7.39	1.30	1.34
1	1A	574	C	N1-C6	-7.39	1.32	1.37
1	1A	1632	A	N7-C5	-7.37	1.34	1.39
1	1A	527	C	N1-C6	-7.34	1.32	1.37
1	1A	2587	A	N3-C4	-7.34	1.30	1.34
32	1a	926	G	N7-C5	-7.33	1.34	1.39
1	1A	2392	A	N9-C4	-7.33	1.33	1.37
1	2A	1782	C	N1-C6	-7.33	1.32	1.37
1	1A	2272	U	C2-N3	-7.32	1.32	1.37
32	1a	828	A	N9-C4	-7.30	1.33	1.37
1	1A	2061	G	C6-N1	-7.29	1.34	1.39
1	1A	685	A	N3-C4	-7.26	1.30	1.34
1	1A	1217	C	N1-C6	-7.26	1.32	1.37
1	2A	1471	A	N9-C4	7.25	1.42	1.37
1	1A	2319	G	N7-C5	-7.24	1.34	1.39
1	2A	1991	U	C2-N3	-7.18	1.32	1.37
1	2A	1815	A	N3-C4	-7.17	1.30	1.34
1	1A	184	C	N1-C6	-7.17	1.32	1.37
1	1A	16	G	N3-C4	-7.16	1.30	1.35
1	1A	2618	G	C6-N1	-7.15	1.34	1.39
1	1A	1847	A	N9-C4	7.09	1.42	1.37
1	1A	1224	C	N1-C6	-7.09	1.32	1.37
1	1A	1661	G	N9-C8	-7.09	1.32	1.37
1	1A	751	A	N3-C4	-7.09	1.30	1.34
1	2A	2616	C	N1-C6	-7.08	1.32	1.37
1	1A	1430	C	N3-C4	-7.07	1.29	1.33
1	1A	2078	C	N1-C6	-7.07	1.32	1.37
1	1A	536	A	N3-C4	-7.02	1.30	1.34
1	1A	2505	G	C2-N3	-7.01	1.27	1.32
1	1A	2621	A	N9-C4	-7.00	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2419	U	C2-N3	-6.99	1.32	1.37
1	1A	503	A	N3-C4	-6.99	1.30	1.34
1	1A	1938	A	N3-C4	-6.98	1.30	1.34
1	2A	1674	G	C6-N1	-6.94	1.34	1.39
1	1A	1002	G	C2-N3	-6.93	1.27	1.32
1	1A	2346	A	N3-C4	-6.92	1.30	1.34
1	1A	1196	C	N1-C6	-6.91	1.33	1.37
1	1A	793	A	N3-C4	-6.90	1.30	1.34
1	1A	1802	A	N9-C4	-6.88	1.33	1.37
1	2A	958	U	C2-N3	6.88	1.42	1.37
1	1A	1315	C	N1-C6	-6.85	1.33	1.37
32	1a	810	C	N1-C6	-6.84	1.33	1.37
1	1A	2015	A	N3-C4	-6.82	1.30	1.34
1	2A	687	C	N3-C4	-6.80	1.29	1.33
1	2A	2821	A	N9-C4	-6.76	1.33	1.37
1	1A	764	A	N7-C5	-6.76	1.35	1.39
1	1A	119	A	N9-C4	-6.73	1.33	1.37
1	1A	2431	U	C2-N3	-6.72	1.33	1.37
1	1A	73	A	C6-N1	-6.71	1.30	1.35
1	1A	1363	C	N3-C4	-6.69	1.29	1.33
1	1A	2048	G	N3-C4	-6.68	1.30	1.35
1	1A	2377	A	N9-C4	-6.68	1.33	1.37
1	1A	2615	U	C2-N3	-6.67	1.33	1.37
1	2A	652(A)	A	N9-C4	6.67	1.41	1.37
1	1A	956	G	C6-O6	6.67	1.30	1.24
1	1A	1213	A	N3-C4	-6.66	1.30	1.34
32	2a	346	G	C2-N3	6.66	1.38	1.32
1	1A	2453	A	C5-C4	-6.64	1.34	1.38
1	1A	323	G	C6-N1	-6.64	1.34	1.39
32	2a	768	A	N9-C4	-6.64	1.33	1.37
1	1A	2225	A	N9-C4	-6.63	1.33	1.37
1	1A	1786	A	N3-C4	-6.62	1.30	1.34
1	1A	529	A	C5-C6	-6.59	1.35	1.41
1	1A	2588	G	C6-N1	-6.58	1.34	1.39
1	1A	1245	G	N7-C5	-6.58	1.35	1.39
1	1A	2711	A	N9-C4	-6.58	1.33	1.37
1	1A	197	A	N9-C4	-6.56	1.33	1.37
32	1a	250	A	N9-C4	6.56	1.41	1.37
1	2A	1802	A	N9-C4	-6.55	1.33	1.37
4	1E	163	GLU	CG-CD	6.53	1.61	1.51
1	1A	2730	C	N1-C6	-6.51	1.33	1.37
1	1A	127	A	C5-C6	-6.51	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2765	A	N7-C5	-6.51	1.35	1.39
1	1A	1254	A	N9-C4	-6.51	1.33	1.37
1	1A	673	C	N1-C6	-6.50	1.33	1.37
1	1A	2578	G	C5-C4	-6.48	1.33	1.38
1	1A	822	U	N1-C2	-6.48	1.32	1.38
1	1A	472	A	N9-C4	-6.45	1.33	1.37
32	2a	768	A	N3-C4	-6.45	1.30	1.34
1	1A	802	A	N7-C5	-6.43	1.35	1.39
1	1A	1573	G	N9-C4	-6.42	1.32	1.38
1	2A	738	G	C6-N1	-6.42	1.35	1.39
1	1A	793	A	C6-N1	-6.41	1.31	1.35
1	2A	1978	A	N3-C4	-6.41	1.31	1.34
1	2A	1638	C	N1-C6	-6.40	1.33	1.37
1	1A	478	A	N7-C5	-6.37	1.35	1.39
1	1A	783	A	C6-N6	-6.37	1.28	1.33
1	2A	780	G	N7-C5	-6.36	1.35	1.39
1	1A	1187	G	N1-C2	-6.36	1.32	1.37
1	1A	2621	A	C5-C4	-6.36	1.34	1.38
1	1A	668	G	C6-N1	-6.35	1.35	1.39
1	1A	2015	A	N9-C4	-6.35	1.34	1.37
1	1A	911	A	N7-C5	-6.35	1.35	1.39
32	1a	346	G	C6-N1	6.33	1.44	1.39
1	1A	2027	G	C6-N1	-6.32	1.35	1.39
1	1A	2607	G	C6-N1	-6.31	1.35	1.39
1	1A	2516	G	N7-C5	-6.31	1.35	1.39
1	1A	2069	G	C6-N1	-6.31	1.35	1.39
32	1a	814	A	N7-C5	-6.30	1.35	1.39
1	1A	2333	A	N9-C8	-6.29	1.32	1.37
1	2A	1372	U	C2-N3	6.29	1.42	1.37
1	1A	525	U	C2-N3	-6.28	1.33	1.37
1	1A	1239	G	N7-C5	-6.28	1.35	1.39
1	1A	975(A)	G	N9-C4	-6.28	1.32	1.38
1	1A	1224	C	N3-C4	-6.28	1.29	1.33
1	1A	1674	G	N9-C8	-6.28	1.33	1.37
1	2A	222	A	N9-C4	-6.28	1.34	1.37
1	1A	1573	G	N3-C4	-6.27	1.31	1.35
1	2A	1721	G	N3-C4	6.26	1.39	1.35
1	1A	793	A	C5-C6	-6.26	1.35	1.41
1	1A	722	A	N9-C4	-6.24	1.34	1.37
1	1A	2319	G	N3-C4	-6.24	1.31	1.35
6	2G	167	GLU	CG-CD	6.22	1.61	1.51
32	2a	975	A	N9-C4	-6.22	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2574	G	C6-N1	-6.21	1.35	1.39
1	1A	2607	G	N3-C4	-6.20	1.31	1.35
1	1A	750	A	C6-N1	-6.18	1.31	1.35
1	1A	975	C	N1-C6	-6.17	1.33	1.37
1	1A	790	C	N3-C4	6.17	1.38	1.33
1	1A	85	G	C5-C4	-6.17	1.34	1.38
1	1A	297	C	N1-C6	-6.17	1.33	1.37
1	1A	2019	A	C5-C6	-6.16	1.35	1.41
1	1A	1786	A	N9-C4	-6.16	1.34	1.37
1	1A	2057	A	N7-C5	-6.15	1.35	1.39
1	1A	2586	C	N1-C6	-6.15	1.33	1.37
1	1A	184	C	N3-C4	-6.15	1.29	1.33
1	1A	2019	A	N7-C5	-6.15	1.35	1.39
1	1A	2026	C	N1-C6	-6.14	1.33	1.37
1	1A	454	A	N7-C5	-6.14	1.35	1.39
1	1A	698	C	N1-C6	-6.14	1.33	1.37
2	2B	26	A	N9-C4	6.14	1.41	1.37
1	1A	1995	U	N1-C2	-6.13	1.33	1.38
1	2A	735	A	N7-C5	-6.13	1.35	1.39
1	1A	2627	G	N7-C5	-6.12	1.35	1.39
1	1A	793	A	N7-C5	-6.12	1.35	1.39
1	1A	228	A	C5-C6	-6.12	1.35	1.41
1	1A	2013	A	C6-N1	-6.12	1.31	1.35
1	1A	2853	C	N1-C6	-6.11	1.33	1.37
1	1A	581	C	N1-C6	-6.10	1.33	1.37
1	1A	1984	G	N9-C8	-6.09	1.33	1.37
1	1A	2609	U	C2-N3	-6.08	1.33	1.37
32	2a	1093	A	N9-C4	6.08	1.41	1.37
1	1A	2604	U	N1-C6	-6.07	1.32	1.38
1	2A	2589	A	N9-C4	-6.07	1.34	1.37
1	1A	739	G	C5-C6	-6.06	1.36	1.42
1	1A	1008	C	C4-C5	-6.06	1.38	1.43
1	1A	1367	A	C6-N6	-6.06	1.29	1.33
1	1A	2589	A	C5-C4	-6.06	1.34	1.38
1	1A	1671	U	N3-C4	-6.05	1.33	1.38
1	1A	2621	A	N7-C5	-6.05	1.35	1.39
1	1A	2328	A	C6-N1	-6.04	1.31	1.35
1	1A	2823	A	C6-N1	-6.04	1.31	1.35
1	1A	1672	C	N1-C6	-6.03	1.33	1.37
32	2a	415	A	N9-C4	6.03	1.41	1.37
1	1A	15	G	C2-N3	-6.03	1.27	1.32
1	1A	1283	G	N9-C8	-6.03	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	58	G	N7-C5	-6.02	1.35	1.39
1	1A	1274	A	N7-C5	-6.02	1.35	1.39
1	2A	1669	A	N3-C4	-6.00	1.31	1.34
1	1A	1952	A	N3-C4	-6.00	1.31	1.34
1	2A	381	G	N3-C4	-6.00	1.31	1.35
32	1a	787	A	N9-C4	-5.99	1.34	1.37
1	2A	1652	A	C6-N1	-5.99	1.31	1.35
1	1A	2410	G	C5-C4	-5.99	1.34	1.38
1	1A	2247	A	N7-C5	-5.99	1.35	1.39
1	2A	1965	C	N3-C4	5.98	1.38	1.33
1	1A	2245	U	C2-N3	-5.98	1.33	1.37
1	1A	1253	A	N9-C8	-5.97	1.32	1.37
1	1A	1954	G	N7-C5	-5.97	1.35	1.39
1	2A	866	A	N3-C4	5.97	1.38	1.34
1	1A	191	A	N9-C4	-5.97	1.34	1.37
30	18	34	TRP	CB-CG	-5.97	1.39	1.50
1	1A	79	G	N7-C5	-5.96	1.35	1.39
1	1A	2225	A	N3-C4	-5.96	1.31	1.34
1	1A	1434	A	C6-N1	-5.95	1.31	1.35
27	15	59	GLU	CG-CD	5.95	1.60	1.51
1	2A	2617	C	N1-C6	-5.95	1.33	1.37
1	1A	2198	A	N9-C4	-5.95	1.34	1.37
1	1A	460	A	C6-N1	-5.94	1.31	1.35
1	2A	2378	A	C6-N6	5.94	1.38	1.33
1	2A	1040	C	N1-C2	5.93	1.46	1.40
1	2A	675	A	N3-C4	-5.92	1.31	1.34
1	1A	597	U	N1-C2	-5.92	1.33	1.38
1	1A	330	A	N9-C4	-5.92	1.34	1.37
1	1A	1268	A	C6-N1	-5.92	1.31	1.35
1	1A	1067	A	N9-C4	5.92	1.41	1.37
1	1A	1799	G	N9-C8	-5.91	1.33	1.37
1	1A	2078	C	N1-C2	-5.91	1.34	1.40
32	1a	926	G	C5-C6	-5.91	1.36	1.42
32	2a	753	A	N3-C4	-5.91	1.31	1.34
1	1A	841	A	N9-C4	-5.91	1.34	1.37
1	2A	1934	C	N3-C4	-5.90	1.29	1.33
1	1A	1638	C	N1-C6	-5.90	1.33	1.37
31	19	11	CYS	CB-SG	-5.90	1.72	1.81
1	1A	2414	G	N7-C5	-5.89	1.35	1.39
1	2A	807	U	C2-N3	5.88	1.41	1.37
1	2A	2451	A	N3-C4	-5.88	1.31	1.34
1	2A	2002	G	C8-N7	-5.87	1.27	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1021	A	N3-C4	-5.87	1.31	1.34
1	1A	2057	A	N9-C8	-5.87	1.33	1.37
1	2A	6	A	N9-C4	5.87	1.41	1.37
1	1A	579	G	N9-C4	-5.87	1.33	1.38
32	1a	1447	A	N9-C4	5.87	1.41	1.37
1	1A	2319	G	C5-C6	-5.86	1.36	1.42
1	1A	85	G	N9-C4	-5.86	1.33	1.38
1	1A	460	A	N3-C4	-5.86	1.31	1.34
1	2A	2600	A	N3-C4	-5.86	1.31	1.34
1	1A	2333	A	N7-C5	-5.85	1.35	1.39
1	1A	2730	C	N3-C4	-5.85	1.29	1.33
1	2A	1985	G	N9-C8	-5.85	1.33	1.37
1	1A	1941	C	N1-C6	-5.85	1.33	1.37
1	1A	2676	C	N3-C4	-5.85	1.29	1.33
1	1A	1032	A	N9-C4	-5.85	1.34	1.37
1	1A	341	G	C6-N1	-5.84	1.35	1.39
1	1A	2587	A	N9-C4	-5.84	1.34	1.37
1	1A	201	C	N1-C6	-5.84	1.33	1.37
1	1A	1308	A	C6-N1	-5.84	1.31	1.35
1	1A	1638	C	C4-C5	-5.83	1.38	1.43
1	1A	2055	C	N1-C6	5.83	1.40	1.37
32	1a	1465	C	N1-C6	-5.83	1.33	1.37
1	1A	1603	A	N3-C4	-5.83	1.31	1.34
1	1A	570	G	C6-O6	-5.82	1.19	1.24
1	1A	85	G	N3-C4	-5.82	1.31	1.35
1	1A	788	A	N7-C5	-5.82	1.35	1.39
32	1a	814	A	N9-C4	-5.82	1.34	1.37
1	2A	392	C	N3-C4	-5.82	1.29	1.33
1	1A	2588	G	N1-C2	-5.81	1.33	1.37
1	2A	2598	A	C6-N6	-5.80	1.29	1.33
1	1A	1904	G	N9-C8	-5.80	1.33	1.37
1	1A	571	A	N9-C4	-5.80	1.34	1.37
1	2A	218	A	N9-C4	-5.80	1.34	1.37
1	1A	2393	A	N3-C4	-5.79	1.31	1.34
1	1A	685	A	C6-N1	-5.79	1.31	1.35
1	2A	2029	G	N7-C5	-5.79	1.35	1.39
32	1a	1493	A	N9-C4	5.78	1.41	1.37
1	1A	733	G	C8-N7	-5.78	1.27	1.30
1	1A	1393	A	C5-C4	-5.78	1.34	1.38
1	1A	2080	G	N9-C8	-5.78	1.33	1.37
1	1A	829	A	N9-C4	-5.77	1.34	1.37
1	1A	2764	A	N9-C4	-5.77	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1759	A	C6-N1	-5.77	1.31	1.35
1	1A	1753	G	N7-C5	-5.77	1.35	1.39
1	1A	642	G	N3-C4	-5.77	1.31	1.35
1	1A	1099	G	N3-C4	5.77	1.39	1.35
32	1a	1515	C	N1-C6	-5.77	1.33	1.37
1	1A	454	A	N9-C4	-5.77	1.34	1.37
1	1A	1570	A	N9-C4	-5.77	1.34	1.37
1	1A	1661	G	C5-C4	-5.76	1.34	1.38
1	1A	2032	G	C5-C6	-5.76	1.36	1.42
1	2A	1313	U	N1-C2	-5.76	1.33	1.38
1	2A	2362	G	N7-C5	5.75	1.42	1.39
1	2A	2061	G	C5-C6	-5.74	1.36	1.42
1	2A	2573	C	C2-N3	5.74	1.40	1.35
1	1A	631	A	N7-C5	-5.74	1.35	1.39
1	2A	2801(A)	A	N9-C4	5.74	1.41	1.37
1	1A	1605	C	N1-C6	-5.74	1.33	1.37
1	1A	804	A	N3-C4	-5.73	1.31	1.34
1	1A	432	A	N7-C5	-5.72	1.35	1.39
1	1A	1219	G	N9-C4	-5.72	1.33	1.38
1	1A	2742	C	N1-C6	-5.72	1.33	1.37
1	1A	2823	A	N3-C4	-5.72	1.31	1.34
1	1A	2032	G	C8-N7	-5.72	1.27	1.30
1	1A	1198	U	C2-O2	-5.72	1.17	1.22
1	1A	1131	G	N1-C2	-5.71	1.33	1.37
1	1A	1312	U	C2-N3	-5.71	1.33	1.37
1	1A	2450	A	C5-C4	-5.71	1.34	1.38
1	1A	1403	C	N3-C4	-5.70	1.29	1.33
1	1A	780	G	N9-C8	-5.69	1.33	1.37
1	1A	2407	G	N3-C4	-5.69	1.31	1.35
1	1A	125	G	C5-C4	-5.68	1.34	1.38
1	2A	1032	A	N9-C4	-5.68	1.34	1.37
2	2B	26	A	C5-C4	5.68	1.42	1.38
1	1A	668	G	N1-C2	-5.68	1.33	1.37
1	1A	799	G	N3-C4	-5.68	1.31	1.35
1	1A	1165	U	N3-C4	-5.68	1.33	1.38
1	1A	1367	A	N3-C4	-5.68	1.31	1.34
1	1A	2078	C	N3-C4	-5.67	1.29	1.33
1	1A	1266	G	N7-C5	5.67	1.42	1.39
1	1A	390	A	N9-C4	-5.67	1.34	1.37
1	1A	1439	A	N9-C4	-5.66	1.34	1.37
1	2A	1970	A	N3-C4	-5.66	1.31	1.34
1	1A	1268	A	N3-C4	-5.65	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1348	G	C5-C4	-5.65	1.34	1.38
1	1A	2790	A	N9-C4	5.65	1.41	1.37
1	1A	118	A	C5-C4	-5.65	1.34	1.38
1	1A	1938	A	N9-C4	-5.65	1.34	1.37
1	1A	2598	A	N9-C4	5.65	1.41	1.37
1	1A	673	C	N3-C4	5.64	1.38	1.33
1	2A	2722	G	C6-N1	-5.64	1.35	1.39
1	1A	1566	A	N3-C4	5.64	1.38	1.34
42	2k	119	CYS	CB-SG	-5.64	1.72	1.81
1	1A	2039	C	C4-C5	-5.63	1.38	1.43
1	1A	2238	G	N9-C8	-5.63	1.33	1.37
1	1A	945	A	C8-N7	-5.63	1.27	1.31
12	1Q	109	VAL	CB-CG2	-5.63	1.41	1.52
1	2A	2393	A	N9-C4	-5.63	1.34	1.37
1	2A	1274	A	N9-C4	-5.62	1.34	1.37
1	1A	579	G	C5-C4	-5.62	1.34	1.38
1	1A	1135	C	N3-C4	-5.62	1.30	1.33
11	2P	98	GLU	CG-CD	5.62	1.60	1.51
1	1A	1938	A	N7-C5	-5.61	1.35	1.39
32	1a	965	A	N9-C4	-5.61	1.34	1.37
1	1A	799	G	C5-C4	-5.61	1.34	1.38
1	1A	2001	A	C5-C4	-5.61	1.34	1.38
1	1A	1665	A	N7-C5	-5.61	1.35	1.39
1	1A	2718	G	N7-C5	-5.61	1.35	1.39
1	1A	2738	A	N9-C4	-5.61	1.34	1.37
1	2A	503	A	N3-C4	-5.61	1.31	1.34
1	1A	2678	C	N1-C6	-5.60	1.33	1.37
1	1A	1937	A	N9-C4	-5.60	1.34	1.37
1	1A	1010	A	N9-C4	-5.60	1.34	1.37
1	1A	1177	A	N9-C4	5.60	1.41	1.37
1	1A	469	G	N7-C5	-5.59	1.35	1.39
1	1A	207	A	N9-C4	-5.59	1.34	1.37
1	1A	778	G	N7-C5	-5.59	1.35	1.39
1	1A	2020	A	C6-N1	-5.59	1.31	1.35
1	1A	669	G	C5-C6	-5.59	1.36	1.42
1	1A	954	G	C6-N1	-5.59	1.35	1.39
1	1A	1627	G	N1-C2	-5.58	1.33	1.37
1	1A	514	A	N9-C8	-5.58	1.33	1.37
1	1A	1142(A)	A	N9-C4	-5.58	1.34	1.37
1	1A	2033	A	C6-N1	-5.58	1.31	1.35
1	1A	1210	A	N3-C4	-5.58	1.31	1.34
1	1A	2737	G	C5-C4	-5.58	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2609	U	N1-C6	-5.57	1.32	1.38
1	1A	1801	G	N7-C5	-5.57	1.35	1.39
1	1A	2801(A)	A	N9-C4	5.57	1.41	1.37
1	1A	2640	G	N3-C4	-5.57	1.31	1.35
1	1A	449	A	N3-C4	-5.57	1.31	1.34
1	1A	2641	G	C5-C4	-5.57	1.34	1.38
1	1A	2823	A	N7-C5	-5.57	1.35	1.39
1	1A	693	C	N1-C6	-5.57	1.33	1.37
1	1A	189	G	N9-C8	-5.56	1.33	1.37
1	1A	189	G	N7-C5	-5.56	1.35	1.39
1	1A	801	G	N7-C5	-5.56	1.35	1.39
1	1A	2626	C	N1-C6	-5.56	1.33	1.37
1	1A	1601	G	N7-C5	-5.56	1.35	1.39
1	2A	676	A	N3-C4	5.56	1.38	1.34
1	1A	428	A	N7-C5	-5.55	1.35	1.39
1	1A	663	G	N3-C4	-5.55	1.31	1.35
8	2I	108	THR	CA-CB	5.54	1.67	1.53
1	1A	2013	A	C5-C4	-5.53	1.34	1.38
1	1A	2621	A	N9-C8	-5.52	1.33	1.37
1	1A	1643	G	C6-N1	-5.52	1.35	1.39
1	1A	2162	G	N9-C4	5.52	1.42	1.38
1	1A	2244	U	C2-O2	-5.52	1.17	1.22
1	1A	632	A	C6-N1	-5.51	1.31	1.35
1	1A	2493	U	N3-C4	-5.51	1.33	1.38
1	1A	832	G	N7-C5	-5.51	1.35	1.39
1	1A	2063	C	N1-C2	-5.51	1.34	1.40
1	1A	2616	C	N3-C4	-5.51	1.30	1.33
1	1A	1091	G	N9-C4	5.51	1.42	1.38
1	1A	614(C)	A	N9-C4	-5.50	1.34	1.37
1	1A	2505	G	C5-C6	-5.50	1.36	1.42
1	1A	2006	C	N3-C4	-5.49	1.30	1.33
1	1A	2454	G	N3-C4	-5.49	1.31	1.35
32	2a	346	G	N9-C4	5.49	1.42	1.38
1	2A	1067	A	N9-C4	5.48	1.41	1.37
32	1a	1429	C	N1-C6	-5.48	1.33	1.37
1	1A	1785	A	C5-C6	-5.48	1.36	1.41
1	1A	786	C	N1-C6	-5.47	1.33	1.37
1	1A	103	A	C6-N6	5.47	1.38	1.33
1	1A	975(A)	G	N9-C8	-5.47	1.34	1.37
1	1A	614(C)	A	N3-C4	-5.47	1.31	1.34
1	1A	16	G	C6-N1	-5.46	1.35	1.39
1	1A	1404	C	N3-C4	-5.46	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2088	G	C6-O6	5.46	1.29	1.24
1	1A	2431	U	N3-C4	-5.45	1.33	1.38
1	1A	2511	U	N3-C4	-5.45	1.33	1.38
1	1A	508	G	N9-C4	-5.45	1.33	1.38
1	1A	803	U	C2-N3	-5.45	1.33	1.37
1	1A	2510	C	N1-C6	-5.45	1.33	1.37
1	1A	242	G	N9-C4	-5.45	1.33	1.38
1	1A	939	G	C5-C4	-5.45	1.34	1.38
1	2A	351	G	N9-C4	5.44	1.42	1.38
1	2A	1045	A	N3-C4	5.44	1.38	1.34
1	2A	2848	G	N9-C8	-5.44	1.34	1.37
1	1A	759	G	N7-C5	-5.44	1.35	1.39
1	1A	1802	A	N7-C5	-5.43	1.35	1.39
1	2A	189	G	N9-C8	-5.43	1.34	1.37
2	1B	83	G	N9-C8	-5.43	1.34	1.37
1	1A	525	U	N1-C2	-5.42	1.33	1.38
1	1A	2000	G	N7-C5	-5.42	1.35	1.39
32	1a	1415	G	N7-C5	-5.42	1.35	1.39
1	1A	782	A	N9-C4	-5.41	1.34	1.37
1	1A	2259	G	C6-N1	5.41	1.43	1.39
1	1A	1187	G	C6-N1	-5.41	1.35	1.39
1	1A	1676	A	N9-C4	-5.40	1.34	1.37
1	2A	1637	A	N3-C4	-5.40	1.31	1.34
1	2A	2058	A	N7-C5	-5.40	1.36	1.39
1	1A	2078	C	C2-N3	-5.40	1.31	1.35
1	1A	1393	A	C6-N1	-5.39	1.31	1.35
1	1A	1854	A	N9-C4	-5.39	1.34	1.37
1	1A	236	C	C2-O2	-5.39	1.19	1.24
1	1A	2331	G	N9-C4	-5.39	1.33	1.38
1	1A	2834	G	N9-C8	-5.39	1.34	1.37
1	2A	2155	G	N7-C5	5.38	1.42	1.39
1	1A	799	G	C6-N1	-5.38	1.35	1.39
1	1A	942	G	N9-C8	-5.38	1.34	1.37
1	1A	1825	A	C6-N1	-5.38	1.31	1.35
1	1A	326	G	N9-C8	-5.38	1.34	1.37
1	1A	2680	C	C4-C5	-5.38	1.38	1.43
1	2A	2441	C	N1-C6	-5.38	1.33	1.37
1	1A	503	A	N9-C4	-5.38	1.34	1.37
20	1Y	76	CYS	CB-SG	-5.38	1.73	1.81
1	2A	1696	G	C5-C4	-5.38	1.34	1.38
1	1A	735	A	C5-C6	-5.38	1.36	1.41
32	2a	1286	A	N9-C4	5.37	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	684	G	C6-N1	-5.37	1.35	1.39
1	1A	781	A	C5-C4	-5.37	1.34	1.38
1	2A	2296	U	N1-C2	5.37	1.43	1.38
1	1A	1577	C	N3-C4	-5.36	1.30	1.33
1	1A	1009	A	N7-C5	-5.36	1.36	1.39
32	1a	327	A	N9-C4	-5.36	1.34	1.37
1	2A	207	A	N3-C4	-5.35	1.31	1.34
1	2A	779	U	C2-O2	-5.35	1.17	1.22
27	25	49	CYS	CB-SG	-5.35	1.73	1.81
4	1E	151	TYR	CE2-CZ	5.35	1.45	1.38
1	1A	1375	C	N1-C6	-5.34	1.33	1.37
32	2a	715	A	N3-C4	-5.34	1.31	1.34
1	1A	1424	G	N3-C4	-5.34	1.31	1.35
1	1A	2042	A	N9-C4	-5.34	1.34	1.37
1	1A	1616	A	C6-N1	-5.34	1.31	1.35
1	1A	2020	A	N7-C5	-5.34	1.36	1.39
1	2A	2451	A	N9-C4	-5.34	1.34	1.37
1	1A	1027	A	N9-C4	-5.33	1.34	1.37
32	2a	1028	C	N1-C6	5.33	1.40	1.37
1	2A	1689	A	N9-C4	-5.33	1.34	1.37
1	1A	589	C	N1-C6	-5.33	1.33	1.37
1	1A	1927	A	N9-C4	-5.33	1.34	1.37
32	1a	1084	G	N9-C4	5.33	1.42	1.38
1	2A	2764	A	N9-C4	-5.32	1.34	1.37
1	1A	2493	U	C2-N3	-5.32	1.34	1.37
1	2A	2695	C	N1-C6	-5.32	1.33	1.37
1	1A	1021	A	N7-C5	-5.32	1.36	1.39
1	1A	470	A	N3-C4	-5.31	1.31	1.34
1	1A	2623	G	C5-C4	-5.31	1.34	1.38
1	2A	189	G	C5-C4	-5.31	1.34	1.38
1	2A	2009	G	C5-C4	-5.31	1.34	1.38
1	1A	394	A	C6-N1	-5.31	1.31	1.35
1	2A	801	G	N9-C4	-5.31	1.33	1.38
1	1A	594	U	C2-N3	-5.30	1.34	1.37
1	2A	783	A	N7-C5	-5.30	1.36	1.39
1	1A	1216	G	N9-C8	-5.30	1.34	1.37
1	1A	1554	A	N9-C4	-5.30	1.34	1.37
1	1A	2589	A	C6-N6	5.30	1.38	1.33
1	1A	239	U	C2-N3	-5.29	1.34	1.37
1	1A	271(Y)	U	C2-N3	-5.29	1.34	1.37
1	1A	1376	C	N1-C6	-5.29	1.33	1.37
1	1A	201	C	N3-C4	-5.29	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	579	G	N3-C4	-5.29	1.31	1.35
32	2a	1151	A	N9-C4	5.29	1.41	1.37
1	1A	1653	G	C8-N7	-5.29	1.27	1.30
1	1A	1655	A	C5-C6	-5.29	1.36	1.41
1	1A	207	A	C6-N1	5.28	1.39	1.35
1	1A	1603	A	N1-C2	-5.28	1.29	1.34
1	1A	467	G	N9-C4	-5.27	1.33	1.38
1	1A	644	A	N3-C4	-5.26	1.31	1.34
32	1a	558	G	C5-C6	-5.26	1.37	1.42
1	1A	125	G	N9-C4	-5.26	1.33	1.38
1	1A	210	C	N1-C6	-5.26	1.33	1.37
1	1A	1938	A	C6-N1	-5.26	1.31	1.35
1	1A	622	G	N9-C8	-5.25	1.34	1.37
1	1A	1853	A	N9-C4	-5.25	1.34	1.37
1	1A	2036	C	N3-C4	-5.25	1.30	1.33
1	1A	579	G	N7-C5	-5.25	1.36	1.39
1	1A	1212	G	N9-C8	-5.25	1.34	1.37
1	2A	570	G	C2-N3	5.24	1.36	1.32
1	1A	1650	G	C2-N3	-5.24	1.28	1.32
1	1A	2436	G	C2-N3	-5.23	1.28	1.32
1	1A	2835	A	N9-C4	-5.23	1.34	1.37
1	2A	34	C	C4-N4	5.23	1.38	1.33
1	1A	1314	C	N1-C6	-5.23	1.34	1.37
1	1A	2442	C	N3-C4	-5.23	1.30	1.33
1	1A	127	A	C5-C4	-5.22	1.35	1.38
1	2A	2009	G	N1-C2	-5.22	1.33	1.37
1	1A	2449	U	C4-O4	5.22	1.27	1.23
32	1a	50	A	N9-C4	-5.22	1.34	1.37
1	1A	503	A	C5-C4	-5.22	1.35	1.38
1	1A	967	C	N3-C4	-5.22	1.30	1.33
1	1A	1668	A	N7-C5	-5.22	1.36	1.39
1	1A	2041	U	N1-C2	-5.22	1.33	1.38
1	1A	1804	C	N1-C6	-5.21	1.34	1.37
1	2A	777	A	N3-C4	-5.21	1.31	1.34
1	2A	1773	A	C6-N1	-5.21	1.31	1.35
16	1U	69	CYS	CB-SG	-5.21	1.73	1.81
1	1A	2242	G	N7-C5	-5.21	1.36	1.39
1	2A	697	C	N1-C6	-5.21	1.34	1.37
1	1A	2381	C	N3-C4	-5.21	1.30	1.33
1	1A	1900	A	C6-N1	-5.20	1.31	1.35
1	1A	2436	G	N1-C2	-5.20	1.33	1.37
1	1A	2725	A	N3-C4	-5.20	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	260	G	N3-C4	-5.20	1.31	1.35
1	1A	2011	U	N1-C2	-5.20	1.33	1.38
1	1A	2389	G	N1-C2	-5.20	1.33	1.37
32	1a	780	A	N9-C4	-5.20	1.34	1.37
1	1A	1897	G	C5-C6	-5.20	1.37	1.42
1	1A	1553	A	N9-C4	-5.20	1.34	1.37
1	1A	2701	C	N3-C4	-5.20	1.30	1.33
1	1A	776	G	C2-N2	-5.20	1.29	1.34
1	1A	1566	A	C5-C6	5.20	1.45	1.41
1	1A	1617	C	N3-C4	-5.19	1.30	1.33
1	1A	509	C	N1-C6	-5.19	1.34	1.37
1	1A	2038	G	N1-C2	-5.19	1.33	1.37
1	1A	73	A	C5-C4	-5.19	1.35	1.38
1	1A	2514	U	C2-N3	-5.19	1.34	1.37
32	1a	898	G	C6-N1	-5.18	1.35	1.39
1	1A	463	G	N3-C4	-5.18	1.31	1.35
1	1A	677	A	N3-C4	-5.18	1.31	1.34
1	1A	1654	A	N7-C5	-5.18	1.36	1.39
1	1A	2618	G	N1-C2	-5.18	1.33	1.37
1	1A	945	A	N3-C4	5.18	1.38	1.34
1	1A	1972	A	N7-C5	-5.18	1.36	1.39
1	1A	1593	G	N3-C4	-5.17	1.31	1.35
1	1A	2585	U	C4-O4	-5.17	1.19	1.23
1	1A	477	A	C6-N1	-5.17	1.31	1.35
1	1A	1785	A	N7-C5	-5.17	1.36	1.39
1	1A	2002	G	C8-N7	-5.17	1.27	1.30
1	1A	2492	U	N3-C4	-5.17	1.33	1.38
32	1a	1151	A	N9-C4	5.17	1.41	1.37
1	2A	2780	G	N9-C4	-5.17	1.33	1.38
1	1A	1219	G	N3-C4	-5.17	1.31	1.35
32	2a	767	A	N7-C5	-5.17	1.36	1.39
1	1A	1203	G	C5-C6	-5.16	1.37	1.42
1	1A	1354	A	C5-C6	-5.16	1.36	1.41
1	2A	1780	A	N3-C4	-5.16	1.31	1.34
36	2e	122	GLU	CG-CD	5.16	1.59	1.51
1	2A	1268	A	C6-N1	-5.16	1.31	1.35
2	2B	57	A	N7-C5	5.16	1.42	1.39
1	2A	2822	G	N9-C8	-5.16	1.34	1.37
1	1A	933	A	N9-C4	-5.16	1.34	1.37
1	1A	571	A	C5-C4	-5.15	1.35	1.38
1	1A	597	U	N1-C6	-5.15	1.33	1.38
32	1a	1278	U	N1-C2	5.15	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2496	C	N1-C6	-5.15	1.34	1.37
1	2A	1691	C	N3-C4	-5.15	1.30	1.33
1	1A	2430	A	C6-N1	-5.14	1.31	1.35
1	1A	2627	G	C5-C6	-5.14	1.37	1.42
1	1A	2004	G	N9-C4	-5.14	1.33	1.38
1	1A	57	C	N1-C2	-5.14	1.35	1.40
1	1A	236	C	N3-C4	-5.14	1.30	1.33
1	1A	964	C	N1-C6	-5.13	1.34	1.37
1	1A	73	A	N3-C4	-5.12	1.31	1.34
1	1A	2040	C	N1-C6	-5.12	1.34	1.37
1	1A	2746	U	C2-N3	-5.12	1.34	1.37
2	1B	27	C	N1-C6	-5.12	1.34	1.37
32	1a	782	A	N9-C4	-5.12	1.34	1.37
1	1A	2534	A	N9-C4	5.11	1.41	1.37
1	2A	1619	G	C2-N3	-5.11	1.28	1.32
1	1A	36	G	N9-C8	-5.11	1.34	1.37
1	1A	1189	A	C5-C4	-5.11	1.35	1.38
1	1A	83	G	N3-C4	5.11	1.39	1.35
1	1A	593	G	N7-C5	-5.11	1.36	1.39
1	1A	1960	A	N9-C4	-5.11	1.34	1.37
1	2A	1978	A	N9-C4	-5.11	1.34	1.37
1	2A	2446	G	C6-N1	-5.11	1.35	1.39
1	1A	783	A	C5-C6	-5.10	1.36	1.41
1	1A	920	G	N7-C5	-5.10	1.36	1.39
1	2A	329	G	N9-C4	5.10	1.42	1.38
1	1A	1244	G	N3-C4	-5.10	1.31	1.35
1	1A	1294	U	N1-C2	-5.10	1.33	1.38
1	1A	2829	C	N1-C6	-5.09	1.34	1.37
1	2A	2577	A	N3-C4	-5.09	1.31	1.34
1	1A	2445	G	C6-N1	-5.09	1.35	1.39
1	1A	663	G	C2-N3	-5.09	1.28	1.32
1	1A	838	C	N1-C6	-5.08	1.34	1.37
1	1A	466	A	C6-N1	-5.08	1.31	1.35
1	2A	528	A	N7-C5	-5.08	1.36	1.39
1	1A	473	G	C6-N1	-5.08	1.35	1.39
1	1A	1073	A	N9-C4	5.08	1.40	1.37
1	1A	1547	C	N1-C6	-5.08	1.34	1.37
1	1A	651	G	C2-N3	-5.08	1.28	1.32
1	1A	1633	G	C6-O6	-5.08	1.19	1.24
1	1A	85	G	N9-C8	-5.08	1.34	1.37
1	1A	980	A	N9-C4	-5.08	1.34	1.37
1	1A	1332	G	N7-C5	-5.08	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1424	G	C6-N1	-5.08	1.35	1.39
1	1A	2662	A	N7-C5	-5.07	1.36	1.39
1	1A	606	U	C2-N3	-5.07	1.34	1.37
1	1A	54	G	N7-C5	-5.07	1.36	1.39
1	1A	789	A	N7-C5	-5.07	1.36	1.39
1	2A	10	G	C6-N1	5.07	1.43	1.39
1	1A	568	U	C4-O4	-5.06	1.19	1.23
1	1A	1275	A	N7-C5	-5.06	1.36	1.39
1	1A	1367	A	C6-N1	-5.06	1.32	1.35
32	2a	715	A	N9-C4	-5.06	1.34	1.37
1	2A	947	G	N9-C4	-5.06	1.33	1.38
1	2A	2365	G	C2-N3	5.06	1.36	1.32
1	1A	578	A	C6-N1	-5.06	1.32	1.35
1	2A	795	C	N3-C4	-5.06	1.30	1.33
32	2a	299	G	C6-O6	-5.06	1.19	1.24
1	1A	2678	C	N3-C4	-5.06	1.30	1.33
1	2A	100	G	N9-C4	5.06	1.42	1.38
1	1A	655	A	N9-C4	-5.05	1.34	1.37
32	2a	1137	C	N1-C6	5.05	1.40	1.37
1	1A	76	C	N1-C6	-5.05	1.34	1.37
1	1A	1777	U	N1-C6	-5.05	1.33	1.38
1	1A	382	G	C5-C4	-5.05	1.34	1.38
1	1A	983	A	N9-C4	-5.05	1.34	1.37
1	1A	975(A)	G	C5-C4	-5.05	1.34	1.38
1	1A	2032	G	C5-C4	-5.05	1.34	1.38
1	2A	783	A	N3-C4	-5.05	1.31	1.34
1	1A	516	C	C4-C5	-5.04	1.39	1.43
1	1A	784	A	N7-C5	-5.04	1.36	1.39
1	1A	1216	G	N7-C5	-5.04	1.36	1.39
1	1A	1323	U	N1-C2	-5.04	1.34	1.38
1	1A	643	A	N3-C4	-5.04	1.31	1.34
1	1A	2222	G	N9-C4	-5.04	1.33	1.38
1	1A	1291	C	N3-C4	-5.04	1.30	1.33
1	1A	2247	A	N9-C8	-5.04	1.33	1.37
1	2A	26	G	N7-C5	-5.04	1.36	1.39
32	1a	885	G	C2-N3	-5.03	1.28	1.32
32	1a	772	U	N1-C2	-5.03	1.34	1.38
32	1a	279	A	N9-C4	-5.03	1.34	1.37
1	1A	577	G	C6-N1	-5.03	1.36	1.39
1	1A	1558	A	N3-C4	-5.03	1.31	1.34
1	1A	2261	C	N3-C4	-5.03	1.30	1.33
1	2A	959	A	N7-C5	-5.03	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2247	A	N3-C4	-5.03	1.31	1.34
1	2A	1675	C	N1-C6	-5.03	1.34	1.37
1	1A	1619	G	N7-C5	-5.02	1.36	1.39
1	1A	992	C	N1-C6	-5.02	1.34	1.37
1	1A	2081	C	N1-C6	-5.02	1.34	1.37
1	1A	1889	A	C5-C4	-5.02	1.35	1.38
1	2A	1632	A	N7-C5	-5.02	1.36	1.39
1	2A	1777	U	N3-C4	-5.02	1.33	1.38
1	1A	1212	G	N3-C4	-5.01	1.31	1.35
1	1A	1821	A	N7-C5	-5.01	1.36	1.39
1	1A	1469	A	N9-C4	-5.01	1.34	1.37
1	1A	1789	A	N9-C4	-5.01	1.34	1.37
1	2A	12	U	N1-C2	5.01	1.43	1.38
1	2A	459	U	C2-N3	-5.01	1.34	1.37
1	1A	2453	A	P-O5'	-5.01	1.54	1.59
2	2B	66	A	N9-C4	5.01	1.40	1.37
32	2a	1278	U	N1-C2	5.01	1.43	1.38
1	1A	236	C	C2-N3	-5.00	1.31	1.35
1	1A	450	G	C6-O6	-5.00	1.19	1.24
1	1A	1665	A	N9-C4	-5.00	1.34	1.37
1	1A	2438	U	N1-C6	-5.00	1.33	1.38
1	2A	412	A	N9-C4	-5.00	1.34	1.37
1	1A	37	C	N3-C4	-5.00	1.30	1.33
1	2A	1990	C	C2-O2	-5.00	1.20	1.24

All (9271) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2319	G	C6-C5-N7	-21.39	117.57	130.40
1	1A	2061	G	O5'-P-OP2	-19.75	87.00	110.70
1	1A	673	C	C5-C4-N4	-18.70	107.11	120.20
1	1A	673	C	N3-C4-C5	17.52	128.91	121.90
1	1A	2319	G	N1-C6-O6	17.08	130.15	119.90
1	1A	673	C	C2-N3-C4	-16.96	111.42	119.90
1	1A	1327	C	N1-C2-O2	-16.71	108.88	118.90
1	1A	2506	U	O5'-P-OP2	-16.61	90.75	105.70
1	1A	570	G	N1-C6-O6	-16.40	110.06	119.90
1	2A	453	C	O5'-P-OP1	-16.27	91.05	105.70
1	2A	1975	G	O5'-P-OP2	-15.84	91.45	105.70
32	1a	903	G	O5'-P-OP2	-15.63	91.63	105.70
1	2A	751	A	O5'-P-OP1	-15.61	91.65	105.70
1	1A	2431	U	C5-C6-N1	-15.36	115.02	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2427	C	O5'-P-OP1	-15.21	92.01	105.70
1	1A	739	G	O5'-P-OP1	-15.11	92.10	105.70
1	1A	1270	C	C6-N1-C2	14.82	126.23	120.30
32	2a	893	C	C6-N1-C2	14.69	126.17	120.30
1	1A	529	A	C5-C6-N6	-14.61	112.01	123.70
1	1A	467	G	O5'-P-OP2	-14.55	92.61	105.70
1	1A	202	U	C5-C6-N1	-14.43	115.48	122.70
1	1A	472	A	O5'-P-OP2	-14.38	92.75	105.70
1	1A	2319	G	C2-N3-C4	-14.36	104.72	111.90
1	1A	2319	G	C4-C5-N7	14.34	116.53	110.80
1	1A	807	U	N1-C2-O2	-14.34	112.77	122.80
1	2A	673	C	C2-N3-C4	-14.33	112.73	119.90
1	1A	2374	C	C6-N1-C2	14.26	126.00	120.30
1	1A	2576	G	O5'-P-OP2	-14.23	92.89	105.70
1	1A	807	U	C2-N3-C4	-14.20	118.48	127.00
1	1A	1327	C	C6-N1-C2	-14.18	114.63	120.30
1	1A	1272	A	O5'-P-OP2	-14.13	92.98	105.70
1	1A	2539	C	C6-N1-C2	13.97	125.89	120.30
32	2a	346	G	N3-C4-C5	-13.76	121.72	128.60
32	1a	404	U	N1-C2-O2	13.73	132.41	122.80
1	2A	2084	C	C6-N1-C2	13.68	125.77	120.30
1	1A	1428	C	C6-N1-C2	13.59	125.73	120.30
1	1A	2070	G	O5'-P-OP2	-13.57	93.49	105.70
1	1A	2319	G	C4-N9-C1'	13.55	144.11	126.50
1	1A	582	G	N1-C6-O6	13.54	128.03	119.90
1	1A	122	G	C8-N9-C4	13.47	111.79	106.40
1	1A	1015	G	O5'-P-OP2	-13.47	93.57	105.70
1	1A	2390	U	O5'-P-OP1	-13.46	93.58	105.70
1	1A	2618	G	N1-C6-O6	-13.39	111.87	119.90
1	1A	2331	G	C8-N9-C4	13.37	111.75	106.40
1	2A	1187	G	N1-C6-O6	-13.35	111.89	119.90
1	2A	148	C	C6-N1-C2	13.26	125.60	120.30
1	1A	1313	U	O5'-P-OP1	-13.17	93.85	105.70
1	1A	1655	A	N1-C6-N6	13.16	126.50	118.60
1	2A	801	G	O5'-P-OP2	-13.12	93.89	105.70
1	1A	579	G	N1-C6-O6	13.11	127.77	119.90
1	2A	807	U	C2-N3-C4	-13.07	119.16	127.00
1	1A	1800	C	N3-C4-C5	-13.07	116.67	121.90
1	2A	588	U	O5'-P-OP2	-12.89	94.10	105.70
1	1A	2609	U	C5-C6-N1	-12.85	116.28	122.70
1	2A	2453	A	C8-N9-C4	12.76	110.91	105.80
1	1A	1830	C	N3-C4-C5	12.75	127.00	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2506	U	O5'-P-OP1	12.75	126.00	110.70
2	1B	99	G	C8-N9-C4	12.75	111.50	106.40
1	1A	529	A	N1-C6-N6	12.68	126.21	118.60
1	1A	807	U	N1-C2-N3	12.68	122.50	114.90
1	1A	529	A	C4-C5-N7	12.65	117.02	110.70
32	1a	343	U	C2-N1-C1'	-12.64	102.53	117.70
1	1A	528	A	C8-N9-C4	-12.62	100.75	105.80
1	1A	204	A	N1-C2-N3	12.58	135.59	129.30
1	1A	330	A	C2-N3-C4	-12.53	104.33	110.60
1	1A	228	A	C5-C6-N6	-12.49	113.71	123.70
1	1A	2319	G	C5-N7-C8	-12.45	98.08	104.30
1	1A	2357	U	O5'-P-OP2	-12.40	94.53	105.70
1	1A	1274	A	N1-C6-N6	12.36	126.02	118.60
1	1A	906	G	C5-C6-O6	12.35	136.01	128.60
1	1A	228	A	N1-C6-N6	12.34	126.00	118.60
1	2A	471	A	O5'-P-OP1	-12.32	94.61	105.70
1	2A	610	G	O5'-P-OP2	-12.29	94.64	105.70
1	1A	906	G	C8-N9-C4	-12.27	101.49	106.40
1	2A	1828	G	O5'-P-OP1	-12.27	94.66	105.70
1	1A	1047	G	N3-C4-C5	-12.26	122.47	128.60
1	2A	1076	C	C6-N1-C2	-12.25	115.40	120.30
1	1A	2319	G	N1-C2-N3	12.22	131.23	123.90
1	1A	1607	C	N1-C2-O2	12.20	126.22	118.90
1	1A	2041	U	N1-C2-O2	-12.20	114.26	122.80
32	2a	893	C	N1-C2-O2	12.18	126.21	118.90
1	1A	783	A	C8-N9-C4	-12.18	100.93	105.80
1	1A	948	G	O5'-P-OP2	12.15	125.28	110.70
1	1A	575	A	O5'-P-OP1	-12.14	94.77	105.70
1	1A	1119	C	C6-N1-C2	12.13	125.15	120.30
32	1a	926	G	N1-C6-O6	12.12	127.17	119.90
1	2A	2573	C	N3-C4-N4	12.07	126.45	118.00
1	1A	1672	C	N3-C4-C5	-12.05	117.08	121.90
1	1A	2249	U	N3-C4-O4	-12.05	110.97	119.40
32	1a	533	A	N1-C6-N6	12.05	125.83	118.60
1	1A	941	A	C8-N9-C4	-12.01	101.00	105.80
1	1A	599	G	C8-N9-C4	12.01	111.20	106.40
1	1A	2006	C	O5'-P-OP1	-12.01	94.89	105.70
1	1A	2005	A	O5'-P-OP1	-11.99	94.91	105.70
1	1A	1566	A	N1-C6-N6	-11.95	111.43	118.60
32	2a	346	G	N3-C4-N9	11.94	133.16	126.00
1	2A	1265	A	O5'-P-OP2	-11.92	94.97	105.70
1	2A	2791	C	C6-N1-C2	-11.91	115.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2319	G	C8-N9-C1'	-11.90	111.52	127.00
1	2A	145	G	C8-N9-C4	11.89	111.16	106.40
1	1A	912	C	C6-N1-C2	-11.88	115.55	120.30
1	1A	1327	C	N3-C4-C5	-11.86	117.16	121.90
1	1A	2319	G	C4-C5-C6	11.82	125.89	118.80
1	1A	529	A	C5-N7-C8	-11.81	98.00	103.90
1	1A	2062	A	C8-N9-C4	11.77	110.51	105.80
1	1A	31	C	O5'-P-OP1	-11.76	95.12	105.70
1	2A	2378	A	N1-C6-N6	11.73	125.64	118.60
1	2A	2079	U	O5'-P-OP1	-11.73	95.14	105.70
2	2B	104	U	C5-C6-N1	-11.72	116.84	122.70
1	1A	1231	G	O5'-P-OP1	11.71	124.75	110.70
1	1A	399	G	O5'-P-OP2	-11.71	95.16	105.70
1	2A	673	C	N3-C4-C5	11.70	126.58	121.90
32	1a	338	A	O5'-P-OP1	-11.66	95.20	105.70
1	1A	477	A	O5'-P-OP2	-11.66	95.21	105.70
1	1A	1268	A	N1-C2-N3	11.65	135.12	129.30
1	1A	729	G	N1-C6-O6	11.64	126.89	119.90
1	1A	2721	A	O5'-P-OP1	-11.64	95.22	105.70
1	1A	2036	C	O5'-P-OP1	-11.63	95.23	105.70
2	2B	115	G	C8-N9-C4	11.63	111.05	106.40
1	1A	1678	G	N3-C2-N2	-11.61	111.77	119.90
1	1A	568	U	O5'-P-OP2	-11.61	95.25	105.70
1	1A	945	A	N9-C4-C5	-11.61	101.16	105.80
1	1A	1162	G	N1-C6-O6	-11.60	112.94	119.90
1	1A	228	A	C4-C5-N7	11.58	116.49	110.70
2	1B	102	A	C6-N1-C2	-11.58	111.65	118.60
1	1A	1800	C	C6-N1-C2	-11.57	115.67	120.30
1	1A	2826	A	C8-N9-C4	11.56	110.42	105.80
1	2A	2074	U	O5'-P-OP1	-11.55	95.30	105.70
32	2a	1137	C	C6-N1-C2	-11.55	115.68	120.30
1	2A	2714	G	N1-C6-O6	11.53	126.82	119.90
1	1A	974	G	O5'-P-OP1	-11.52	95.33	105.70
2	2B	6	C	C6-N1-C2	11.51	124.90	120.30
1	1A	45	C	N3-C2-O2	11.51	129.95	121.90
1	1A	1270	C	C5-C6-N1	-11.49	115.25	121.00
1	1A	103	A	C5-C6-N1	-11.48	111.96	117.70
1	1A	1653	G	C8-N9-C1'	-11.47	112.08	127.00
1	2A	2755	C	C5-C6-N1	11.46	126.73	121.00
1	2A	1187	G	C5-C6-O6	11.40	135.44	128.60
1	1A	2431	U	C2-N3-C4	-11.39	120.16	127.00
1	1A	1667	G	O5'-P-OP1	-11.37	95.47	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	738	G	N1-C6-O6	-11.36	113.08	119.90
1	2A	1678	G	C6-C5-N7	-11.35	123.59	130.40
32	1a	404	U	N3-C2-O2	-11.31	114.28	122.20
1	1A	1284	A	N1-C6-N6	11.31	125.39	118.60
1	2A	2578	G	O5'-P-OP1	-11.31	95.52	105.70
1	1A	1970	A	O5'-P-OP2	-11.30	95.53	105.70
1	2A	1639	U	O5'-P-OP2	-11.29	95.54	105.70
1	1A	829	A	C8-N9-C4	11.28	110.31	105.80
1	2A	956	G	N1-C6-O6	11.28	126.67	119.90
1	2A	1124	C	O5'-P-OP1	-11.28	95.55	105.70
1	1A	673	C	O5'-P-OP1	11.24	124.19	110.70
1	1A	906	G	N9-C4-C5	11.22	109.89	105.40
32	1a	226	G	C8-N9-C4	11.20	110.88	106.40
1	1A	1607	C	C2-N1-C1'	11.20	131.12	118.80
1	1A	570	G	C5-C6-N1	11.20	117.10	111.50
1	1A	1130	U	O5'-P-OP1	-11.20	95.62	105.70
1	1A	1455	G	N1-C6-O6	11.18	126.61	119.90
1	2A	2050	C	O5'-P-OP2	-11.18	95.64	105.70
1	1A	2319	G	O4'-C1'-N9	11.17	117.14	108.20
32	1a	897	C	C6-N1-C2	11.17	124.77	120.30
1	1A	1340	U	C2-N3-C4	-11.17	120.30	127.00
32	1a	1530	G	N1-C6-O6	11.17	126.60	119.90
1	1A	226	G	C2-N3-C4	11.14	117.47	111.90
1	2A	2478	A	C8-N9-C4	11.12	110.25	105.80
1	2A	863	A	O5'-P-OP2	-11.09	95.72	105.70
1	1A	999	U	O5'-P-OP2	-11.08	95.73	105.70
1	1A	755	C	N3-C4-C5	-11.08	117.47	121.90
1	1A	391	G	C5-C6-O6	-11.07	121.96	128.60
1	1A	1186	G	C8-N9-C4	11.07	110.83	106.40
1	2A	673	C	C5-C4-N4	-11.05	112.46	120.20
1	2A	945	A	O5'-P-OP1	-11.05	95.75	105.70
1	1A	127	A	C5-C6-N6	-11.05	114.86	123.70
1	1A	1283	G	C8-N9-C4	11.05	110.82	106.40
1	1A	2487	G	N1-C6-O6	11.05	126.53	119.90
1	1A	2319	G	N7-C8-N9	11.01	118.60	113.10
1	1A	2820	A	C2-N3-C4	-11.01	105.10	110.60
1	1A	1814	G	C5-C6-O6	10.99	135.19	128.60
1	1A	729	G	C5-C6-O6	-10.98	122.01	128.60
32	1a	926	G	C6-C5-N7	-10.98	123.81	130.40
1	1A	681	G	N1-C6-O6	10.98	126.49	119.90
1	1A	1222	C	N1-C2-O2	-10.98	112.31	118.90
2	1B	75	G	C6-N1-C2	-10.97	118.52	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1653	G	C4-N9-C1'	10.96	140.74	126.50
1	1A	934	G	C8-N9-C4	10.95	110.78	106.40
1	2A	2610	C	O5'-P-OP1	-10.94	95.86	105.70
32	1a	926	G	C5-C6-O6	-10.92	122.05	128.60
1	2A	1471	A	C8-N9-C4	-10.92	101.43	105.80
1	1A	938	G	O5'-P-OP2	-10.91	95.88	105.70
1	2A	2617	C	N3-C4-C5	-10.91	117.53	121.90
1	1A	698	C	O5'-P-OP2	-10.91	95.88	105.70
1	2A	827	U	N3-C2-O2	10.91	129.83	122.20
1	2A	2453	A	N7-C8-N9	-10.87	108.36	113.80
1	1A	1363	C	O5'-P-OP2	-10.85	95.93	105.70
32	2a	547	A	O5'-P-OP1	-10.84	95.94	105.70
1	2A	1663	C	C6-N1-C2	10.84	124.64	120.30
1	1A	945	A	C8-N9-C4	10.83	110.13	105.80
1	1A	2707	G	C8-N9-C4	10.83	110.73	106.40
1	1A	776	G	N1-C2-N3	10.83	130.40	123.90
1	1A	2040	C	C6-N1-C2	10.82	124.63	120.30
1	1A	1434	A	N1-C6-N6	-10.82	112.11	118.60
1	1A	228	A	C5-N7-C8	-10.81	98.49	103.90
1	1A	2817	G	C8-N9-C4	-10.80	102.08	106.40
32	1a	267	C	O5'-P-OP1	-10.80	95.98	105.70
32	2a	404	U	N1-C2-O2	10.80	130.36	122.80
1	1A	732	C	N1-C2-O2	-10.79	112.43	118.90
1	1A	2607	G	C2-N3-C4	-10.79	106.50	111.90
32	2a	1528	U	O5'-P-OP2	-10.78	96.00	105.70
1	1A	1239	G	N1-C6-O6	10.77	126.36	119.90
1	1A	2576	G	O5'-P-OP1	10.77	123.62	110.70
1	1A	1147	C	O5'-P-OP2	-10.75	96.02	105.70
1	1A	582	G	C5-C6-O6	-10.75	122.15	128.60
1	1A	1655	A	C5-C6-N6	-10.75	115.10	123.70
1	1A	1777	U	C5-C6-N1	-10.74	117.33	122.70
1	1A	1655	A	C8-N9-C4	10.74	110.10	105.80
1	1A	2447	G	C5-C6-O6	-10.73	122.16	128.60
32	2a	346	G	C6-N1-C2	-10.72	118.67	125.10
1	1A	1142(A)	A	O5'-P-OP1	-10.71	96.06	105.70
1	1A	2259	G	N1-C6-O6	10.71	126.33	119.90
1	2A	1200	C	C6-N1-C2	10.70	124.58	120.30
1	2A	1187	G	C8-N9-C4	-10.68	102.13	106.40
1	2A	982	C	C6-N1-C2	-10.67	116.03	120.30
1	2A	1073	A	N1-C6-N6	-10.67	112.20	118.60
1	2A	2319	G	O4'-C1'-N9	10.65	116.72	108.20
1	2A	1031	G	C8-N9-C4	10.64	110.66	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1622	G	N3-C2-N2	-10.64	112.45	119.90
1	1A	2439	A	C8-N9-C4	-10.64	101.55	105.80
1	1A	1993	U	C5-C6-N1	-10.63	117.38	122.70
1	2A	1046	A	O4'-C1'-N9	10.63	116.70	108.20
1	1A	2259	G	C5-C6-O6	-10.63	122.22	128.60
1	1A	1299	G	O5'-P-OP1	-10.63	96.14	105.70
1	1A	231	C	N1-C2-O2	-10.62	112.53	118.90
1	2A	72	U	O5'-P-OP1	-10.62	96.14	105.70
32	2a	1027	C	C6-N1-C2	-10.62	116.05	120.30
1	2A	852	G	O5'-P-OP2	-10.60	96.16	105.70
1	1A	2612	C	N1-C2-O2	10.60	125.26	118.90
1	1A	2881	C	O5'-P-OP1	-10.59	96.17	105.70
1	1A	1817	G	C8-N9-C4	-10.58	102.17	106.40
1	1A	1801	G	N1-C6-O6	10.57	126.24	119.90
32	1a	558	G	C4-C5-N7	10.55	115.02	110.80
1	1A	1655	A	N9-C4-C5	-10.55	101.58	105.80
1	1A	947	G	O5'-P-OP2	-10.53	96.22	105.70
1	1A	1607	C	C6-N1-C1'	-10.53	108.16	120.80
1	2A	97	C	C6-N1-C2	10.51	124.50	120.30
32	2a	21	G	O5'-P-OP1	-10.51	96.24	105.70
1	2A	2427	C	O5'-P-OP1	-10.50	96.25	105.70
1	1A	818	G	C5-C6-O6	-10.49	122.30	128.60
1	1A	856	C	C6-N1-C2	-10.48	116.11	120.30
1	1A	136	G	C8-N9-C4	10.47	110.59	106.40
1	1A	1799	G	C8-N9-C4	10.47	110.59	106.40
1	1A	2518	A	O5'-P-OP2	10.47	123.26	110.70
32	2a	893	C	N3-C4-C5	10.46	126.09	121.90
1	1A	783	A	N1-C6-N6	-10.46	112.33	118.60
1	1A	758	C	O5'-P-OP2	-10.45	96.30	105.70
1	1A	2727	G	O5'-P-OP2	-10.44	96.30	105.70
32	1a	14	U	O5'-P-OP1	-10.45	96.30	105.70
32	2a	1003	G	C8-N9-C4	-10.44	102.22	106.40
1	1A	1622	G	C4-C5-N7	-10.43	106.63	110.80
1	2A	1932	A	N1-C6-N6	10.43	124.86	118.60
1	1A	1676	A	O5'-P-OP2	-10.41	96.33	105.70
1	2A	1122	G	O5'-P-OP2	-10.41	96.33	105.70
1	1A	207	A	N1-C6-N6	10.40	124.84	118.60
1	1A	576	U	O5'-P-OP1	-10.39	96.34	105.70
1	1A	1597	A	O5'-P-OP2	-10.39	96.35	105.70
1	1A	1497	U	C5-C4-O4	10.38	132.13	125.90
1	2A	462	C	C5-C6-N1	-10.37	115.81	121.00
1	1A	62	C	C6-N1-C2	10.37	124.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2735	G	N1-C6-O6	-10.36	113.68	119.90
1	1A	579	G	C5-C6-O6	-10.36	122.38	128.60
1	1A	2627	G	C5-C6-O6	-10.36	122.38	128.60
1	1A	1187	G	C5-C6-N1	10.36	116.68	111.50
32	1a	558	G	C5-C6-O6	-10.36	122.39	128.60
1	2A	906	G	N9-C4-C5	10.35	109.54	105.40
1	1A	2283	C	O5'-P-OP2	-10.34	96.39	105.70
2	1B	118	G	N3-C4-C5	10.34	133.77	128.60
1	1A	737	C	C6-N1-C2	10.34	124.44	120.30
1	1A	392	C	O5'-P-OP1	-10.34	96.40	105.70
1	1A	12	U	N3-C2-O2	-10.33	114.97	122.20
1	2A	1365	A	N1-C6-N6	-10.32	112.41	118.60
1	1A	524	U	O5'-P-OP1	-10.30	96.43	105.70
1	1A	372	G	C5-C6-O6	-10.30	122.42	128.60
1	1A	2430	A	C8-N9-C4	-10.30	101.68	105.80
1	1A	2374	C	C5-C6-N1	-10.29	115.85	121.00
1	1A	122	G	N1-C6-O6	10.29	126.07	119.90
1	1A	1340	U	N1-C2-N3	10.27	121.06	114.90
1	1A	1343	G	C8-N9-C4	-10.27	102.29	106.40
1	1A	1631	C	O5'-P-OP1	-10.27	96.46	105.70
1	1A	763	G	C2-N3-C4	-10.26	106.77	111.90
32	2a	896	C	C6-N1-C2	10.26	124.41	120.30
1	2A	34	C	N3-C4-C5	-10.26	117.80	121.90
32	1a	558	G	N1-C6-O6	10.26	126.05	119.90
1	1A	686	G	C4-C5-N7	10.24	114.90	110.80
1	2A	2726	U	C6-N1-C2	10.24	127.14	121.00
1	1A	1336	A	O5'-P-OP2	-10.23	96.49	105.70
1	2A	1120	G	C8-N9-C4	10.23	110.49	106.40
1	2A	956	G	C5-C6-N1	-10.23	106.39	111.50
1	2A	2585	U	OP1-P-O3'	10.22	127.69	105.20
1	1A	733	G	C8-N9-C4	10.21	110.48	106.40
1	2A	2177	C	N1-C2-O2	10.21	125.02	118.90
2	2B	104	U	C6-N1-C2	10.20	127.12	121.00
32	2a	1432	G	N1-C6-O6	-10.20	113.78	119.90
2	2B	24	G	C5-C6-O6	-10.19	122.49	128.60
1	1A	2699	C	N1-C2-O2	-10.19	112.79	118.90
1	2A	2586	C	O5'-P-OP1	-10.18	96.54	105.70
1	1A	2858	C	O5'-P-OP2	-10.18	96.54	105.70
1	2A	197	A	C5-C6-N6	-10.18	115.56	123.70
1	2A	2244	U	C5-C6-N1	-10.17	117.61	122.70
1	1A	329	G	C8-N9-C4	10.16	110.46	106.40
1	1A	2514	U	C6-N1-C2	10.14	127.09	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	694	U	N3-C2-O2	-10.14	115.10	122.20
1	1A	2505	G	N1-C6-O6	10.14	125.98	119.90
1	1A	1395	A	O5'-P-OP1	-10.14	96.57	105.70
1	1A	2447	G	C6-N1-C2	-10.14	119.02	125.10
32	1a	1529	G	C8-N9-C4	-10.12	102.35	106.40
1	2A	746	A	O5'-P-OP1	-10.12	96.59	105.70
1	1A	1602	U	O5'-P-OP2	10.12	122.84	110.70
1	1A	1814	G	N9-C4-C5	10.12	109.45	105.40
1	1A	2166	G	C5-C6-O6	10.11	134.67	128.60
1	1A	1972	A	N7-C8-N9	10.10	118.85	113.80
32	1a	893	C	N1-C2-O2	10.10	124.96	118.90
1	2A	1325	G	N3-C4-N9	10.10	132.06	126.00
1	1A	1131	G	N3-C2-N2	10.09	126.97	119.90
32	2a	267	C	O5'-P-OP1	-10.09	96.62	105.70
1	1A	2043	C	N3-C4-C5	-10.09	117.86	121.90
1	1A	2591	C	O5'-P-OP1	-10.08	96.62	105.70
1	1A	2612	C	C6-N1-C2	10.08	124.33	120.30
1	2A	127	A	C8-N9-C4	10.08	109.83	105.80
1	1A	1957	C	C6-N1-C2	10.07	124.33	120.30
1	2A	2573	C	C5-C4-N4	-10.07	113.15	120.20
1	2A	2726	U	N3-C2-O2	10.06	129.25	122.20
1	1A	2038	G	N1-C6-O6	-10.06	113.87	119.90
32	2a	483	C	C6-N1-C2	10.06	124.32	120.30
1	1A	1132	A	O5'-P-OP1	-10.05	96.65	105.70
1	1A	1047	G	N3-C4-N9	10.05	132.03	126.00
1	1A	1888	G	N1-C6-O6	10.04	125.93	119.90
1	1A	534	U	C5-C6-N1	-10.04	117.68	122.70
1	1A	598	G	O5'-P-OP2	-10.03	96.67	105.70
1	1A	2487	G	O5'-P-OP1	-10.03	96.67	105.70
2	1B	102	A	N1-C2-N3	10.01	134.30	129.30
1	2A	2413	G	O5'-P-OP2	-10.00	96.70	105.70
32	1a	343	U	N3-C4-O4	-9.99	112.41	119.40
1	2A	2179	C	C6-N1-C2	-9.99	116.31	120.30
1	1A	863	A	O5'-P-OP2	-9.98	96.72	105.70
1	1A	1830	C	C6-N1-C2	9.96	124.29	120.30
1	1A	2439	A	O5'-P-OP2	-9.97	96.73	105.70
1	1A	1651	G	N1-C6-O6	9.96	125.88	119.90
32	1a	615	C	C6-N1-C2	-9.96	116.31	120.30
1	2A	975	C	O5'-P-OP1	-9.95	96.74	105.70
1	1A	2268	A	O5'-P-OP1	-9.95	96.75	105.70
1	1A	2823	A	N1-C2-N3	9.95	134.27	129.30
32	2a	1508	G	O5'-P-OP1	-9.94	96.75	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	244	A	N1-C6-N6	9.93	124.56	118.60
1	2A	330	A	C4-C5-N7	9.93	115.66	110.70
1	2A	330	A	N9-C4-C5	-9.93	101.83	105.80
32	1a	1478	C	C6-N1-C2	9.92	124.27	120.30
1	1A	259	G	N1-C6-O6	9.91	125.85	119.90
1	1A	733	G	N9-C4-C5	-9.90	101.44	105.40
1	1A	2407	G	C5-C6-N1	-9.90	106.55	111.50
1	1A	911	A	N1-C6-N6	9.90	124.54	118.60
32	1a	339	C	C6-N1-C2	9.90	124.26	120.30
1	2A	1759	A	C2-N3-C4	-9.90	105.65	110.60
1	2A	2447	G	O5'-P-OP1	-9.88	96.80	105.70
1	1A	125	G	C8-N9-C4	9.88	110.35	106.40
1	1A	1443	G	O5'-P-OP1	-9.88	96.81	105.70
1	1A	790	C	N3-C4-N4	9.87	124.91	118.00
32	1a	1442(A)	G	C5-C6-O6	-9.87	122.68	128.60
1	1A	528	A	N7-C8-N9	9.86	118.73	113.80
1	1A	1609	A	C8-N9-C4	9.86	109.74	105.80
1	1A	1847	A	O4'-C1'-N9	9.86	116.08	108.20
1	2A	1200	C	C5-C6-N1	-9.86	116.07	121.00
1	1A	194	G	O5'-P-OP2	-9.85	96.83	105.70
1	1A	2440	C	C5-C4-N4	9.84	127.09	120.20
1	1A	676	A	O5'-P-OP2	-9.84	96.84	105.70
1	1A	2062	A	C2-N3-C4	-9.84	105.68	110.60
32	1a	533	A	C5-C6-N6	-9.83	115.83	123.70
32	2a	1420	C	C6-N1-C2	-9.82	116.37	120.30
1	1A	1814	G	N1-C6-O6	-9.82	114.01	119.90
1	2A	1403	C	C6-N1-C2	-9.82	116.37	120.30
2	2B	99	G	N3-C2-N2	-9.82	113.03	119.90
1	1A	2346	A	C6-N1-C2	-9.81	112.71	118.60
1	1A	1936	A	C8-N9-C4	-9.81	101.88	105.80
1	2A	1408	C	N1-C2-O2	-9.81	113.02	118.90
1	1A	960	A	C5-C6-N6	-9.80	115.86	123.70
1	2A	2454	G	OP1-P-OP2	9.80	134.30	119.60
1	1A	2485	G	C8-N9-C4	9.79	110.32	106.40
32	1a	402	G	O5'-P-OP2	-9.79	96.89	105.70
1	2A	1639	U	O5'-P-OP1	9.79	122.44	110.70
1	2A	576	U	O5'-P-OP1	-9.78	96.90	105.70
32	2a	770	C	O5'-P-OP2	-9.78	96.90	105.70
1	2A	330	A	C6-C5-N7	-9.77	125.46	132.30
1	1A	2414	G	C6-C5-N7	-9.77	124.54	130.40
1	1A	1551	C	C6-N1-C2	-9.76	116.40	120.30
1	2A	2375	G	C2-N3-C4	-9.76	107.02	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2618	G	C5-C6-O6	9.75	134.45	128.60
1	1A	2588	G	N1-C6-O6	-9.75	114.05	119.90
1	2A	645	C	N1-C2-O2	9.75	124.75	118.90
1	1A	615	G	N1-C6-O6	-9.74	114.05	119.90
1	1A	1972	A	C8-N9-C4	-9.74	101.90	105.80
1	1A	1825	A	N1-C6-N6	-9.74	112.75	118.60
1	1A	685	A	C8-N9-C4	-9.74	101.91	105.80
1	1A	904	C	N3-C4-N4	-9.73	111.19	118.00
1	1A	1753	G	C6-C5-N7	-9.73	124.56	130.40
1	1A	2406	U	O5'-P-OP2	-9.73	96.95	105.70
1	2A	2516	G	O5'-P-OP2	-9.73	96.95	105.70
1	2A	1008	C	N3-C2-O2	-9.72	115.09	121.90
1	1A	1660	C	N3-C2-O2	-9.72	115.09	121.90
1	1A	2042	A	O5'-P-OP1	-9.72	96.95	105.70
1	2A	2755	C	N3-C4-N4	9.71	124.80	118.00
1	1A	1497	U	N3-C4-O4	-9.70	112.61	119.40
3	1D	48	ARG	NE-CZ-NH1	-9.69	115.45	120.30
1	2A	2760	C	C6-N1-C2	9.69	124.17	120.30
1	1A	2619	C	C6-N1-C2	9.69	124.17	120.30
1	2A	2705	A	C8-N9-C4	9.68	109.67	105.80
1	1A	1965	C	C6-N1-C2	9.68	124.17	120.30
1	1A	39	C	O5'-P-OP2	-9.67	97.00	105.70
1	1A	914	C	O5'-P-OP2	-9.67	97.00	105.70
1	1A	1337	G	OP1-P-O3'	9.67	126.47	105.20
1	2A	2714	G	C5-C6-O6	-9.66	122.80	128.60
1	1A	1696	G	O5'-P-OP2	-9.66	97.01	105.70
32	1a	1466	C	C6-N1-C2	-9.65	116.44	120.30
1	2A	2588	G	C5-C6-N1	-9.65	106.68	111.50
1	1A	122	G	N7-C8-N9	-9.64	108.28	113.10
1	1A	2258	C	N3-C2-O2	-9.63	115.16	121.90
1	2A	12	U	N3-C2-O2	-9.63	115.46	122.20
2	1B	13	A	O5'-P-OP2	-9.62	97.04	105.70
1	1A	202	U	C6-N1-C2	9.62	126.77	121.00
1	1A	204	A	C2-N3-C4	-9.62	105.79	110.60
1	1A	1234	U	O5'-P-OP1	-9.62	97.05	105.70
1	1A	2062	A	N9-C4-C5	-9.61	101.96	105.80
1	1A	1514	U	O5'-P-OP2	-9.60	97.06	105.70
1	1A	2696	U	N3-C2-O2	-9.59	115.49	122.20
1	1A	2445	G	C8-N9-C4	-9.58	102.57	106.40
1	1A	177	G	C5-C6-O6	9.58	134.35	128.60
1	1A	569	U	C5-C6-N1	-9.58	117.91	122.70
32	1a	817	C	C6-N1-C2	9.57	124.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	823	G	C8-N9-C4	9.57	110.23	106.40
32	1a	781	A	C5-C6-N6	-9.56	116.05	123.70
1	1A	2618	G	C8-N9-C4	-9.56	102.58	106.40
1	1A	1612	C	C6-N1-C2	9.56	124.12	120.30
1	1A	2240	C	C6-N1-C2	9.55	124.12	120.30
1	2A	2714	G	C4-C5-N7	9.55	114.62	110.80
1	1A	193	U	C4-C5-C6	9.54	125.43	119.70
1	2A	2346	A	O5'-P-OP1	-9.54	97.11	105.70
1	1A	2088	G	N1-C6-O6	9.54	125.62	119.90
1	1A	2578	G	C5-C6-N1	9.54	116.27	111.50
1	2A	1793	C	N3-C4-C5	9.53	125.71	121.90
1	2A	2408	U	N3-C2-O2	-9.54	115.53	122.20
1	2A	2081	C	C6-N1-C2	9.53	124.11	120.30
1	2A	2789	C	C2-N1-C1'	-9.53	108.32	118.80
1	1A	1801	G	C5-N7-C8	-9.52	99.54	104.30
1	1A	1644	C	C5-C6-N1	-9.52	116.24	121.00
1	2A	2821	A	C2-N3-C4	-9.52	105.84	110.60
1	1A	2567	G	O5'-P-OP1	-9.51	97.14	105.70
1	1A	1609	A	N1-C6-N6	9.50	124.30	118.60
1	2A	26	G	C5-C6-O6	-9.50	122.90	128.60
1	2A	2378	A	C4-C5-C6	9.50	121.75	117.00
1	2A	2244	U	C4-C5-C6	9.49	125.40	119.70
1	2A	2019	A	C8-N9-C4	9.49	109.60	105.80
32	2a	404	U	C2-N1-C1'	9.49	129.09	117.70
1	1A	751	A	C6-N1-C2	-9.49	112.91	118.60
1	1A	2779	U	N3-C2-O2	-9.48	115.56	122.20
1	2A	2711	A	O5'-P-OP1	-9.48	97.17	105.70
1	2A	906	G	C8-N9-C4	-9.47	102.61	106.40
1	1A	623	G	O5'-P-OP2	-9.47	97.18	105.70
1	1A	686	G	C5-C6-O6	-9.46	122.92	128.60
1	1A	1239	G	C6-C5-N7	-9.46	124.72	130.40
1	2A	1599	C	N3-C4-C5	-9.46	118.12	121.90
32	1a	1466	C	N3-C4-C5	-9.43	118.13	121.90
1	2A	1049	C	C6-N1-C2	-9.43	116.53	120.30
32	2a	1499	A	O5'-P-OP2	-9.43	97.21	105.70
1	1A	1259	G	C5-C6-O6	-9.42	122.95	128.60
1	1A	1493	C	C2-N1-C1'	9.41	129.15	118.80
1	2A	866	A	N9-C4-C5	-9.41	102.04	105.80
32	2a	1495	U	N1-C2-O2	9.41	129.39	122.80
1	1A	2001	A	C2-N3-C4	9.40	115.30	110.60
1	2A	979	G	O5'-P-OP1	-9.40	97.24	105.70
1	2A	704	G	C8-N9-C4	-9.40	102.64	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1280	G	C8-N9-C4	9.40	110.16	106.40
32	2a	343	U	C2-N1-C1'	-9.39	106.44	117.70
32	1a	284	G	N1-C6-O6	9.38	125.53	119.90
1	2A	409	C	O5'-P-OP1	-9.38	97.26	105.70
1	1A	132	G	C8-N9-C4	9.37	110.15	106.40
32	1a	1417	G	C5-C6-N1	9.37	116.19	111.50
1	2A	794	G	C8-N9-C4	9.36	110.14	106.40
1	1A	768	G	N1-C6-O6	9.36	125.51	119.90
1	1A	838	C	C4-C5-C6	9.36	122.08	117.40
1	1A	2515	C	O5'-P-OP1	9.35	121.92	110.70
1	1A	749	C	C6-N1-C2	9.35	124.04	120.30
1	1A	226	G	C5-C6-O6	-9.34	122.99	128.60
1	1A	2358	G	C5-C6-O6	-9.34	123.00	128.60
1	1A	1253	A	O5'-P-OP1	-9.34	97.29	105.70
1	1A	2252	G	N9-C4-C5	-9.34	101.66	105.40
1	2A	2439	A	C2-N3-C4	-9.34	105.93	110.60
1	1A	789	A	C4-C5-C6	9.34	121.67	117.00
1	2A	800	A	O5'-P-OP1	-9.34	97.30	105.70
1	2A	1008	C	N1-C2-O2	9.34	124.50	118.90
1	1A	484	C	O5'-P-OP2	-9.33	97.30	105.70
1	1A	2319	G	C5-C6-O6	-9.33	123.00	128.60
1	1A	1125	G	N1-C2-N3	9.33	129.50	123.90
1	1A	1202	C	N3-C2-O2	9.33	128.43	121.90
1	1A	2347	C	O5'-P-OP2	-9.32	97.31	105.70
1	1A	582	G	C4-C5-N7	9.32	114.53	110.80
1	2A	1648	C	O5'-P-OP2	-9.32	97.31	105.70
1	1A	2662	A	C8-N9-C4	-9.32	102.07	105.80
1	1A	2505	G	C5-C6-O6	-9.32	123.01	128.60
1	1A	2319	G	C5-C6-N1	-9.31	106.84	111.50
1	1A	2050	C	N3-C4-C5	-9.31	118.18	121.90
1	1A	1236	G	C8-N9-C4	9.31	110.12	106.40
1	1A	272(H)	C	O5'-P-OP2	-9.30	97.33	105.70
1	1A	2443	C	C6-N1-C2	-9.30	116.58	120.30
1	1A	83	G	N9-C4-C5	-9.30	101.68	105.40
32	1a	784	C	C6-N1-C2	9.30	124.02	120.30
1	1A	968	G	N1-C6-O6	-9.29	114.33	119.90
1	2A	718	A	N1-C6-N6	9.29	124.17	118.60
1	1A	2826	A	N7-C8-N9	-9.28	109.16	113.80
32	1a	1278	U	N1-C2-O2	9.28	129.30	122.80
1	1A	582	G	N9-C4-C5	-9.27	101.69	105.40
1	1A	2433	A	N1-C6-N6	9.27	124.16	118.60
1	1A	2442	C	C5-C6-N1	-9.27	116.36	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	945	A	N1-C6-N6	9.27	124.16	118.60
1	1A	1124	C	O5'-P-OP1	-9.27	97.36	105.70
32	1a	781	A	N1-C6-N6	9.27	124.16	118.60
1	1A	1776	G	O5'-P-OP2	-9.27	97.36	105.70
1	1A	1152	C	C6-N1-C2	9.25	124.00	120.30
32	1a	781	A	N9-C4-C5	-9.25	102.10	105.80
1	1A	226	G	N1-C6-O6	9.25	125.45	119.90
1	1A	1801	G	O5'-P-OP1	-9.24	97.38	105.70
1	1A	2062	A	O5'-P-OP2	-9.24	97.38	105.70
1	1A	2008	C	C6-N1-C2	-9.24	116.60	120.30
1	1A	2590	A	C5-N7-C8	-9.24	99.28	103.90
1	1A	226	G	O4'-C1'-N9	9.24	115.59	108.20
1	1A	1900	A	N1-C6-N6	-9.23	113.06	118.60
1	1A	2054	A	OP2-P-O3'	9.23	125.50	105.20
1	1A	488	G	C4-C5-N7	-9.22	107.11	110.80
1	1A	458	G	N3-C4-N9	-9.22	120.47	126.00
32	1a	794	A	O5'-P-OP2	-9.22	97.40	105.70
1	2A	2295	C	C6-N1-C2	-9.21	116.61	120.30
1	1A	458	G	N9-C4-C5	9.21	109.08	105.40
32	2a	1465	C	C5-C4-N4	-9.21	113.75	120.20
32	1a	1484	C	C6-N1-C2	9.21	123.98	120.30
1	1A	325	G	O5'-P-OP2	-9.20	97.42	105.70
1	1A	1800	C	C5-C4-N4	9.20	126.64	120.20
1	1A	869	G	N1-C6-O6	-9.20	114.38	119.90
1	1A	1695	G	C6-C5-N7	-9.20	124.88	130.40
1	2A	2324	C	N3-C4-C5	9.20	125.58	121.90
1	1A	1186	G	O5'-P-OP2	-9.19	97.43	105.70
1	1A	207	A	C5-N7-C8	-9.19	99.31	103.90
1	1A	2193	G	C8-N9-C4	9.19	110.08	106.40
1	1A	988	A	N1-C6-N6	9.19	124.11	118.60
1	1A	1132	A	N1-C2-N3	9.19	133.89	129.30
32	2a	342	C	C6-N1-C2	-9.19	116.63	120.30
1	1A	391	G	C6-N1-C2	-9.18	119.59	125.10
3	1D	60	ARG	NE-CZ-NH1	-9.18	115.71	120.30
1	2A	382	G	O5'-P-OP1	-9.18	97.44	105.70
1	2A	1109	C	C2-N1-C1'	9.18	128.90	118.80
1	2A	2685	G	N1-C6-O6	-9.18	114.39	119.90
1	1A	1825	A	O5'-P-OP2	-9.18	97.44	105.70
1	1A	2346	A	N1-C2-N3	9.18	133.89	129.30
1	1A	179	G	N1-C6-O6	9.18	125.41	119.90
32	1a	1495	U	N1-C2-O2	9.18	129.23	122.80
32	1a	1084	G	N3-C4-N9	9.18	131.51	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1415	G	N1-C6-O6	9.18	125.41	119.90
1	2A	2032	G	C5-C6-N1	9.18	116.09	111.50
32	1a	1084	G	N3-C4-C5	-9.17	124.02	128.60
1	2A	2019	A	N7-C8-N9	-9.17	109.22	113.80
1	1A	1046	A	C8-N9-C4	-9.17	102.13	105.80
1	2A	430	G	N1-C6-O6	9.17	125.40	119.90
1	1A	579	G	O5'-P-OP1	-9.16	97.45	105.70
1	1A	2354	G	O5'-P-OP2	-9.16	97.45	105.70
1	1A	1817	G	N1-C6-O6	-9.16	114.41	119.90
1	1A	534	U	C5-C4-O4	9.15	131.39	125.90
32	1a	781	A	C4-C5-N7	9.15	115.28	110.70
1	1A	330	A	C5-N7-C8	-9.14	99.33	103.90
1	1A	1002	G	N1-C6-O6	9.14	125.39	119.90
1	1A	642	G	O5'-P-OP2	-9.14	97.47	105.70
1	1A	1657	C	C6-N1-C2	9.14	123.96	120.30
1	2A	738	G	C5-C6-O6	9.14	134.08	128.60
1	1A	755	C	C4-C5-C6	9.13	121.97	117.40
1	1A	1839	G	C8-N9-C1'	-9.13	115.12	127.00
1	2A	2618	G	O5'-P-OP2	-9.13	97.48	105.70
1	2A	12	U	N1-C2-O2	9.13	129.19	122.80
1	1A	1261	C	C6-N1-C2	9.13	123.95	120.30
1	1A	1950	G	O5'-P-OP1	-9.13	97.48	105.70
32	2a	794	A	O5'-P-OP2	-9.13	97.48	105.70
1	1A	673	C	C6-N1-C2	9.13	123.95	120.30
1	1A	2407	G	N1-C6-O6	9.13	125.38	119.90
1	1A	655	A	N7-C8-N9	9.12	118.36	113.80
1	1A	1779	U	O5'-P-OP1	-9.12	97.49	105.70
1	1A	271(W)	G	C5-C6-N1	-9.12	106.94	111.50
1	1A	48	G	C4-C5-N7	-9.12	107.15	110.80
1	1A	2378	A	N1-C6-N6	9.12	124.07	118.60
32	1a	254	G	O5'-P-OP1	-9.12	97.50	105.70
1	1A	485	C	N3-C4-C5	9.11	125.54	121.90
1	1A	2361	A	C2-N3-C4	-9.10	106.05	110.60
1	1A	977	G	C8-N9-C4	9.10	110.04	106.40
32	1a	533	A	C6-C5-N7	-9.09	125.94	132.30
1	1A	1838	C	C6-N1-C2	-9.09	116.67	120.30
1	1A	1343	G	N7-C8-N9	9.08	117.64	113.10
1	1A	1004	C	C6-N1-C2	-9.08	116.67	120.30
1	1A	1011	G	C8-N9-C4	9.08	110.03	106.40
1	1A	1304	C	N3-C4-C5	9.08	125.53	121.90
1	2A	2061	G	C5-C6-O6	-9.07	123.16	128.60
1	1A	1839	G	C4-N9-C1'	9.07	138.29	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1936	A	N7-C8-N9	9.07	118.33	113.80
1	2A	1975	G	O5'-P-OP1	9.07	121.58	110.70
1	1A	686	G	N9-C4-C5	-9.07	101.77	105.40
1	1A	1957	C	C5-C6-N1	-9.07	116.47	121.00
1	2A	383	U	N3-C4-C5	-9.07	109.16	114.60
1	1A	272(E)	G	N1-C6-O6	9.06	125.34	119.90
1	1A	2038	G	C5-C6-O6	9.04	134.03	128.60
1	1A	508	G	N3-C4-N9	-9.04	120.57	126.00
32	2a	404	U	N3-C2-O2	-9.04	115.87	122.20
1	1A	1830	C	C5-C4-N4	-9.04	113.87	120.20
1	2A	541	C	O5'-P-OP1	-9.04	97.56	105.70
1	1A	1863	G	C8-N9-C4	9.04	110.02	106.40
1	1A	2370	G	O5'-P-OP2	-9.04	97.57	105.70
1	2A	582	G	C8-N9-C4	9.04	110.01	106.40
1	2A	2827	C	C6-N1-C2	9.04	123.91	120.30
1	2A	2554	U	O5'-P-OP2	-9.03	97.57	105.70
1	1A	906	G	N1-C6-O6	-9.03	114.48	119.90
1	1A	986	C	C4-C5-C6	-9.03	112.89	117.40
1	2A	197	A	C5-C6-N1	9.03	122.22	117.70
1	2A	614	U	N3-C2-O2	-9.03	115.88	122.20
1	2A	1471	A	N7-C8-N9	9.03	118.31	113.80
1	2A	272	G	N1-C6-O6	9.02	125.31	119.90
1	1A	1753	G	C4-C5-N7	9.02	114.41	110.80
1	1A	1493	C	C6-N1-C1'	-9.02	109.98	120.80
32	2a	345	C	C6-N1-C2	-9.02	116.69	120.30
1	1A	1654	A	O5'-P-OP1	-9.02	97.59	105.70
1	1A	829	A	O5'-P-OP2	-9.01	97.59	105.70
1	1A	1197	G	C8-N9-C4	9.01	110.00	106.40
1	1A	575	A	O5'-P-OP2	9.01	121.51	110.70
1	1A	963	U	O5'-P-OP2	9.01	121.51	110.70
1	1A	1776	G	O5'-P-OP1	9.01	121.51	110.70
1	1A	2517	C	C6-N1-C2	9.01	123.90	120.30
1	1A	2655	G	O4'-C1'-N9	9.01	115.41	108.20
32	1a	558	G	N9-C4-C5	-9.01	101.80	105.40
32	2a	901	A	O5'-P-OP1	-9.01	97.59	105.70
1	2A	548	A	O4'-C1'-N9	9.00	115.40	108.20
1	1A	679	C	C6-N1-C2	8.99	123.90	120.30
1	1A	568	U	N3-C4-C5	8.99	120.00	114.60
32	1a	343	U	C6-N1-C1'	8.99	133.79	121.20
32	2a	791	G	N1-C6-O6	8.99	125.29	119.90
32	2a	487	A	C8-N9-C4	8.98	109.39	105.80
1	2A	381	G	C5-C6-N1	-8.98	107.01	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	391	G	N3-C4-N9	8.97	131.38	126.00
1	1A	453	C	O5'-P-OP1	-8.97	97.62	105.70
1	1A	2246	G	C5-C6-O6	-8.97	123.22	128.60
1	1A	2107	C	C6-N1-C2	-8.97	116.71	120.30
1	1A	2589	A	C8-N9-C4	8.97	109.39	105.80
1	2A	329	G	C8-N9-C4	-8.97	102.81	106.40
1	1A	1272	A	N1-C2-N3	8.97	133.78	129.30
1	1A	2439	A	N7-C8-N9	8.96	118.28	113.80
1	1A	2627	G	C4-C5-N7	8.96	114.38	110.80
1	2A	518	G	C8-N9-C4	-8.96	102.82	106.40
1	1A	2048	G	C5-C6-N1	-8.96	107.02	111.50
1	1A	79	G	C5-C6-O6	-8.95	123.23	128.60
1	2A	430	G	C5-C6-O6	-8.95	123.23	128.60
1	1A	206	U	C5-C6-N1	-8.94	118.23	122.70
1	2A	95	G	N1-C6-O6	8.94	125.26	119.90
1	1A	180	G	C5-C6-O6	-8.94	123.24	128.60
1	1A	285	C	C6-N1-C2	8.94	123.87	120.30
1	1A	1046	A	O4'-C1'-N9	8.94	115.35	108.20
32	2a	1397	C	C2-N1-C1'	8.93	128.63	118.80
1	1A	95	G	C8-N9-C4	-8.93	102.83	106.40
1	1A	1367	A	C6-N1-C2	-8.93	113.24	118.60
1	2A	331	A	C8-N9-C4	-8.93	102.23	105.80
1	1A	611	C	C6-N1-C2	8.93	123.87	120.30
1	1A	1286	A	N1-C6-N6	-8.93	113.25	118.60
1	1A	715	G	N3-C4-N9	8.92	131.35	126.00
32	1a	1278	U	N3-C2-O2	-8.92	115.95	122.20
1	1A	1814	G	C8-N9-C4	-8.92	102.83	106.40
1	2A	1224	C	C6-N1-C2	8.92	123.87	120.30
32	2a	558	G	O5'-P-OP1	-8.91	97.68	105.70
32	2a	231	G	O5'-P-OP2	-8.91	97.68	105.70
1	1A	1428	C	C5-C6-N1	-8.91	116.55	121.00
1	2A	193	U	N1-C2-N3	8.90	120.24	114.90
1	1A	963	U	O5'-P-OP1	-8.90	97.69	105.70
1	2A	50	U	N1-C2-N3	-8.90	109.56	114.90
1	2A	2062	A	C5-C6-N6	-8.90	116.58	123.70
32	1a	818	G	N9-C4-C5	8.89	108.96	105.40
32	1a	756	C	C6-N1-C2	8.89	123.86	120.30
1	1A	2705	A	N1-C6-N6	8.89	123.93	118.60
1	1A	2848	G	C4-C5-N7	-8.89	107.24	110.80
1	2A	213	A	C8-N9-C4	8.89	109.36	105.80
1	1A	818	G	N1-C6-O6	8.89	125.23	119.90
1	1A	1671	U	N3-C4-O4	-8.89	113.18	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	650	C	N3-C4-C5	-8.88	118.35	121.90
1	2A	2010	G	C5-C6-N1	-8.88	107.06	111.50
1	1A	860	U	C5-C4-O4	8.88	131.23	125.90
1	2A	330	A	C5-N7-C8	-8.88	99.46	103.90
32	2a	346	G	C5-C6-N1	8.88	115.94	111.50
1	1A	1342	A	C8-N9-C4	8.88	109.35	105.80
1	1A	2407	G	C2-N3-C4	-8.88	107.46	111.90
1	1A	1363	C	N3-C4-N4	-8.87	111.79	118.00
32	1a	1137	C	C6-N1-C2	-8.87	116.75	120.30
1	2A	2372	G	N1-C6-O6	8.87	125.22	119.90
1	1A	1020	A	N9-C4-C5	8.87	109.35	105.80
1	1A	683	C	C6-N1-C2	8.86	123.84	120.30
1	1A	733	G	N3-C4-N9	8.86	131.32	126.00
1	1A	1312	U	O5'-P-OP1	-8.86	97.72	105.70
1	2A	1264	G	C5-C6-N1	-8.86	107.07	111.50
1	2A	2822	G	C8-N9-C1'	-8.86	115.48	127.00
32	1a	1525	G	C4-C5-N7	8.86	114.34	110.80
32	1a	896	C	C6-N1-C2	8.86	123.84	120.30
1	1A	1047	G	C2-N3-C4	8.85	116.33	111.90
1	2A	2073	C	C6-N1-C2	-8.85	116.76	120.30
32	2a	346	G	C2-N3-C4	8.85	116.33	111.90
1	1A	579	G	N3-C2-N2	-8.85	113.70	119.90
1	1A	1230	C	C6-N1-C2	8.85	123.84	120.30
1	2A	784	A	O4'-C1'-N9	8.85	115.28	108.20
1	1A	1283	G	N7-C8-N9	-8.84	108.68	113.10
1	2A	2442	C	N3-C4-C5	-8.84	118.36	121.90
1	1A	193	U	N3-C4-C5	-8.84	109.30	114.60
1	1A	2719	G	O5'-P-OP2	-8.84	97.75	105.70
1	1A	1308	A	C8-N9-C4	-8.84	102.27	105.80
32	2a	343	U	C5-C4-O4	8.84	131.20	125.90
1	1A	732	C	N3-C4-C5	-8.83	118.37	121.90
1	1A	1683	C	N1-C2-O2	-8.83	113.60	118.90
1	2A	30	G	O5'-P-OP2	-8.83	97.76	105.70
1	1A	127	A	N1-C6-N6	8.82	123.89	118.60
1	1A	1255	U	N1-C2-O2	8.82	128.97	122.80
32	1a	1502	A	O5'-P-OP2	-8.81	97.77	105.70
1	1A	800	A	N1-C6-N6	-8.81	113.31	118.60
1	1A	1816	G	O5'-P-OP1	-8.80	97.78	105.70
1	1A	2521	C	C6-N1-C2	8.80	123.82	120.30
1	1A	2628	C	C6-N1-C2	8.80	123.82	120.30
1	2A	182	A	O5'-P-OP1	-8.80	97.78	105.70
1	1A	2823	A	C8-N9-C4	-8.80	102.28	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	120	U	O5'-P-OP1	-8.79	97.79	105.70
1	1A	2250	G	N1-C6-O6	-8.79	114.62	119.90
1	2A	1190	G	N3-C4-C5	-8.79	124.20	128.60
32	1a	376	G	C8-N9-C4	8.79	109.92	106.40
1	1A	985	C	C4-C5-C6	-8.78	113.01	117.40
1	1A	777	A	N9-C4-C5	8.78	109.31	105.80
1	1A	2607	G	C8-N9-C4	-8.78	102.89	106.40
1	1A	2616	C	N3-C4-N4	-8.78	111.86	118.00
1	1A	1756	G	C4-C5-N7	-8.78	107.29	110.80
1	1A	1259	G	N1-C6-O6	8.77	125.16	119.90
32	1a	572	A	C8-N9-C4	8.77	109.31	105.80
32	1a	1412	C	C6-N1-C2	8.77	123.81	120.30
1	2A	462	C	O5'-P-OP2	-8.77	97.81	105.70
32	2a	1495	U	N3-C2-O2	-8.77	116.06	122.20
1	1A	619	G	C5-C6-O6	-8.76	123.34	128.60
1	2A	94(A)	G	C8-N9-C4	-8.76	102.89	106.40
1	2A	1391	U	O5'-P-OP1	-8.76	97.81	105.70
1	1A	860	U	N3-C4-O4	-8.76	113.27	119.40
1	1A	1692	U	C5-C6-N1	-8.76	118.32	122.70
32	2a	926	G	N3-C4-N9	8.76	131.26	126.00
1	2A	1667	G	N1-C6-O6	8.76	125.15	119.90
1	1A	323	G	N1-C6-O6	-8.75	114.65	119.90
1	2A	251	A	C4-C5-C6	8.75	121.38	117.00
1	2A	1351	C	C6-N1-C2	-8.75	116.80	120.30
1	1A	572	A	C8-N9-C4	-8.75	102.30	105.80
32	2a	1522	U	O5'-P-OP2	-8.75	97.83	105.70
1	1A	1494	A	C8-N9-C4	-8.75	102.30	105.80
32	2a	880	C	O5'-P-OP2	-8.75	97.83	105.70
1	1A	911	A	C5-C6-N6	-8.74	116.71	123.70
2	1B	75	G	N3-C2-N2	-8.74	113.78	119.90
1	2A	50	U	C6-N1-C2	8.73	126.24	121.00
1	2A	214	G	O4'-C1'-N9	8.73	115.18	108.20
1	1A	1795	C	C6-N1-C2	8.72	123.79	120.30
1	2A	956	G	C2-N3-C4	-8.72	107.54	111.90
1	1A	1795	C	N3-C4-C5	8.72	125.39	121.90
1	1A	1455	G	C5-C6-O6	-8.72	123.37	128.60
1	1A	1678	G	N1-C6-O6	8.72	125.13	119.90
1	1A	2068	U	C5-C6-N1	-8.71	118.34	122.70
32	1a	1058	G	C8-N9-C4	8.72	109.89	106.40
1	2A	1340	U	C5-C4-O4	-8.71	120.67	125.90
32	1a	1077	G	O5'-P-OP2	-8.71	97.86	105.70
1	2A	704	G	N9-C4-C5	8.71	108.88	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2003	G	N1-C6-O6	8.71	125.12	119.90
1	1A	103	A	C8-N9-C4	8.70	109.28	105.80
1	1A	595	C	O5'-P-OP2	-8.70	97.87	105.70
1	1A	1342	A	N1-C6-N6	8.70	123.82	118.60
1	2A	74	A	O5'-P-OP1	8.70	121.14	110.70
32	2a	728	A	N1-C6-N6	8.70	123.82	118.60
1	1A	751	A	N9-C4-C5	8.69	109.28	105.80
2	2B	79	C	C6-N1-C2	-8.69	116.83	120.30
1	2A	573	G	OP1-P-O3'	8.68	124.30	105.20
1	2A	1828	G	O5'-P-OP2	8.68	121.12	110.70
1	1A	478	A	C8-N9-C4	-8.68	102.33	105.80
1	1A	2397	G	C8-N9-C4	-8.68	102.93	106.40
1	2A	791	C	O5'-P-OP2	-8.68	97.89	105.70
1	2A	819	A	O5'-P-OP1	-8.68	97.89	105.70
32	2a	530	G	N3-C4-N9	8.68	131.21	126.00
1	1A	1309	G	N1-C6-O6	8.68	125.11	119.90
1	1A	1653	G	C4-C5-C6	8.67	124.00	118.80
1	1A	2036	C	N3-C4-N4	-8.67	111.93	118.00
1	2A	1268	A	C2-N3-C4	-8.67	106.27	110.60
1	1A	1265	A	O5'-P-OP2	-8.66	97.90	105.70
32	1a	398	C	C6-N1-C2	8.66	123.77	120.30
1	2A	655	A	C8-N9-C4	-8.66	102.33	105.80
1	1A	2589	A	N7-C8-N9	-8.66	109.47	113.80
1	2A	749	C	N1-C2-O2	8.66	124.09	118.90
1	2A	2177	C	N3-C2-O2	-8.66	115.84	121.90
1	1A	1198	U	N1-C2-N3	8.65	120.09	114.90
1	1A	945	A	C5-C6-N6	-8.65	116.78	123.70
32	1a	964	A	C8-N9-C4	8.65	109.26	105.80
1	2A	1930	G	C4-C5-N7	-8.65	107.34	110.80
1	2A	2324	C	C6-N1-C2	8.65	123.76	120.30
1	1A	448	U	N3-C2-O2	-8.64	116.15	122.20
1	2A	518	G	N3-C4-C5	-8.64	124.28	128.60
1	1A	2116	G	O4'-C1'-N9	8.64	115.11	108.20
1	2A	1964	G	C2-N3-C4	-8.64	107.58	111.90
1	1A	2644	G	N1-C6-O6	8.64	125.08	119.90
1	1A	45	C	C4-C5-C6	-8.63	113.08	117.40
1	1A	48	G	N9-C4-C5	8.63	108.85	105.40
1	2A	624	C	O5'-P-OP1	-8.63	97.93	105.70
1	1A	207	A	C4-C5-N7	8.62	115.01	110.70
1	1A	446	G	N9-C4-C5	-8.62	101.95	105.40
1	1A	2011	U	N3-C2-O2	8.62	128.24	122.20
32	1a	576	G	C4-N9-C1'	8.62	137.71	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	127	G	N3-C4-C5	8.62	132.91	128.60
1	2A	2822	G	N3-C4-N9	8.61	131.17	126.00
1	1A	126	A	C6-N1-C2	8.61	123.77	118.60
1	1A	2329	G	C8-N9-C4	8.61	109.84	106.40
32	2a	442	C	C6-N1-C2	-8.61	116.86	120.30
1	1A	1783	A	OP1-P-O3'	8.61	124.13	105.20
1	2A	521	G	N1-C6-O6	8.61	125.06	119.90
1	2A	1230	C	C6-N1-C2	8.61	123.74	120.30
1	2A	1620	G	N1-C6-O6	8.60	125.06	119.90
1	1A	1817	G	N9-C4-C5	8.60	108.84	105.40
2	2B	74	U	C5-C4-O4	8.60	131.06	125.90
1	1A	690	G	C8-N9-C4	8.60	109.84	106.40
32	2a	525	C	C5-C6-N1	8.59	125.30	121.00
32	2a	530	G	N3-C4-C5	-8.59	124.31	128.60
32	1a	1530	G	C5-C6-O6	-8.59	123.45	128.60
1	1A	1340	U	C5-C4-O4	-8.59	120.75	125.90
1	2A	2032	G	N1-C6-O6	-8.59	114.75	119.90
1	1A	2258	C	N1-C2-O2	8.58	124.05	118.90
1	2A	2061	G	C4-C5-N7	8.58	114.23	110.80
1	1A	28	A	OP1-P-OP2	-8.58	106.73	119.60
1	1A	1644	C	C6-N1-C2	8.58	123.73	120.30
1	2A	452	G	N3-C4-N9	8.58	131.15	126.00
1	2A	118	A	O5'-P-OP1	-8.57	97.98	105.70
1	1A	634	C	O5'-P-OP2	-8.57	97.98	105.70
1	1A	1707	G	C8-N9-C4	8.57	109.83	106.40
1	1A	1838	C	O5'-P-OP1	-8.57	97.99	105.70
1	1A	1274	A	C6-C5-N7	-8.57	126.30	132.30
1	1A	1684	C	O5'-P-OP2	-8.57	97.99	105.70
1	1A	2201	C	O5'-P-OP2	-8.57	97.99	105.70
1	2A	2442	C	C4-C5-C6	8.57	121.68	117.40
1	2A	1187	G	N9-C4-C5	8.56	108.83	105.40
1	1A	2466	C	C6-N1-C2	8.56	123.72	120.30
1	1A	127	A	N9-C4-C5	-8.56	102.38	105.80
1	1A	985	C	C5-C6-N1	8.56	125.28	121.00
1	1A	910	A	C8-N9-C4	8.56	109.22	105.80
1	1A	2373	G	O5'-P-OP1	-8.56	98.00	105.70
1	1A	2718	G	N1-C6-O6	8.56	125.04	119.90
1	2A	391	G	C8-N9-C1'	-8.56	115.88	127.00
1	1A	1695	G	N1-C6-O6	8.55	125.03	119.90
1	1A	713	G	C8-N9-C4	8.55	109.82	106.40
1	1A	934	G	N7-C8-N9	-8.55	108.83	113.10
1	1A	673	C	N3-C4-N4	8.55	123.98	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2407	G	C6-C5-N7	-8.54	125.27	130.40
1	1A	267	C	N3-C4-C5	8.54	125.32	121.90
1	1A	2052	G	C5-C6-O6	-8.54	123.47	128.60
1	1A	2283	C	N3-C2-O2	8.54	127.88	121.90
1	2A	2726	U	N1-C2-N3	-8.54	109.78	114.90
1	2A	1409	C	O5'-P-OP2	-8.54	98.02	105.70
1	1A	531	C	O5'-P-OP1	-8.53	98.02	105.70
1	2A	840	C	N3-C4-C5	-8.53	118.49	121.90
1	2A	1957	C	C6-N1-C2	-8.53	116.89	120.30
1	1A	910	A	N9-C4-C5	-8.53	102.39	105.80
1	1A	2331	G	N7-C8-N9	-8.53	108.83	113.10
1	1A	663	G	C8-N9-C4	-8.53	102.99	106.40
1	1A	2464	C	N3-C2-O2	8.53	127.87	121.90
1	1A	2088	G	C4-C5-N7	8.53	114.21	110.80
1	2A	498	G	C5-C6-O6	-8.53	123.48	128.60
32	2a	577	G	C8-N9-C4	8.53	109.81	106.40
32	2a	1499	A	C8-N9-C4	8.53	109.21	105.80
1	1A	2730	C	C5-C6-N1	-8.52	116.74	121.00
1	2A	659	C	C6-N1-C2	8.52	123.71	120.30
1	1A	2789	C	C2-N1-C1'	-8.52	109.43	118.80
1	1A	1613	G	C2-N3-C4	-8.52	107.64	111.90
1	1A	1812	A	C5-C6-N1	8.52	121.96	117.70
1	2A	2523	G	O5'-P-OP2	-8.52	98.04	105.70
1	1A	201	C	C5-C6-N1	-8.51	116.75	121.00
1	1A	975	C	O5'-P-OP1	-8.51	98.04	105.70
1	1A	650	C	C6-N1-C2	-8.51	116.90	120.30
1	1A	713	G	C2-N3-C4	-8.51	107.65	111.90
32	2a	912	C	C6-N1-C2	8.51	123.70	120.30
1	1A	713	G	N1-C6-O6	8.50	125.00	119.90
1	1A	1617	C	N3-C4-C5	8.50	125.30	121.90
1	2A	1927	A	O5'-P-OP2	-8.50	98.05	105.70
1	2A	1331	A	N1-C6-N6	-8.49	113.50	118.60
1	1A	433	C	C6-N1-C2	-8.49	116.90	120.30
32	1a	893	C	C6-N1-C2	8.49	123.70	120.30
1	1A	79	G	N1-C6-O6	8.49	124.99	119.90
1	1A	312	G	O5'-P-OP1	-8.49	98.06	105.70
1	1A	860	U	O5'-P-OP2	-8.49	98.06	105.70
1	1A	1680	U	N3-C4-O4	-8.49	113.46	119.40
1	1A	1801	G	N7-C8-N9	8.49	117.34	113.10
1	1A	2700	C	N3-C4-C5	8.49	125.30	121.90
1	2A	2567	G	N1-C6-O6	8.49	124.99	119.90
1	1A	906	G	N3-C4-N9	-8.48	120.91	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2011	U	N3-C2-O2	8.48	128.14	122.20
1	1A	109	G	N1-C6-O6	-8.48	114.81	119.90
3	1D	52	ARG	NE-CZ-NH2	8.48	124.54	120.30
1	1A	1641	A	N1-C2-N3	8.48	133.54	129.30
2	1B	89	G	C5-C6-N1	-8.48	107.26	111.50
1	2A	80	G	N1-C6-O6	-8.48	114.81	119.90
1	1A	2056	G	C5-C6-O6	-8.47	123.52	128.60
1	1A	2499	C	N3-C4-C5	-8.47	118.51	121.90
1	2A	2488	A	C8-N9-C4	8.47	109.19	105.80
1	1A	733	G	N7-C8-N9	-8.47	108.86	113.10
32	1a	1530	G	C4-C5-N7	8.47	114.19	110.80
1	2A	2495	G	N1-C6-O6	8.46	124.97	119.90
1	1A	1228	G	C8-N9-C4	8.45	109.78	106.40
1	1A	1312	U	C5-C4-O4	8.45	130.97	125.90
1	2A	1781	C	O5'-P-OP2	-8.45	98.09	105.70
1	1A	569	U	C2-N3-C4	-8.45	121.93	127.00
1	1A	1372	U	N3-C4-O4	8.45	125.31	119.40
1	1A	2027	G	C5-N7-C8	8.45	108.52	104.30
1	1A	2827	C	C6-N1-C2	8.45	123.68	120.30
1	1A	1309	G	C5-C6-N1	-8.45	107.28	111.50
1	1A	261	G	N1-C6-O6	8.44	124.97	119.90
32	1a	841	U	C2-N1-C1'	8.44	127.83	117.70
1	1A	663	G	N3-C2-N2	-8.44	113.99	119.90
1	1A	1254	A	N1-C2-N3	8.44	133.52	129.30
1	1A	1573	G	N3-C4-C5	8.44	132.82	128.60
1	1A	2244	U	N1-C2-N3	8.44	119.96	114.90
1	1A	1137	G	N1-C6-O6	8.44	124.96	119.90
1	1A	1203	G	C4-C5-N7	8.44	114.17	110.80
1	1A	2447	G	N3-C2-N2	-8.44	114.00	119.90
1	2A	1906	G	O5'-P-OP1	-8.44	98.11	105.70
1	1A	177	G	C4-C5-N7	-8.43	107.43	110.80
1	1A	335	C	N3-C4-C5	-8.43	118.53	121.90
1	1A	777	A	C8-N9-C4	-8.43	102.43	105.80
1	2A	2088	G	C5-C6-N1	-8.43	107.28	111.50
1	1A	910	A	N1-C6-N6	8.43	123.66	118.60
1	2A	621	A	N1-C6-N6	-8.43	113.54	118.60
1	1A	2107	C	N3-C4-C5	-8.43	118.53	121.90
1	2A	1780	A	N1-C2-N3	8.43	133.51	129.30
32	2a	1244	C	C6-N1-C2	-8.42	116.93	120.30
1	1A	2592	G	O5'-P-OP1	-8.42	98.12	105.70
1	1A	619	G	N1-C6-O6	8.42	124.95	119.90
1	2A	1476	C	C6-N1-C2	-8.42	116.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	926	G	C4-C5-N7	8.41	114.16	110.80
1	1A	678	C	C5-C6-N1	-8.41	116.80	121.00
1	1A	1219	G	O5'-P-OP1	8.41	120.79	110.70
1	2A	26	G	N1-C6-O6	8.41	124.94	119.90
1	1A	2613	U	N3-C2-O2	-8.40	116.32	122.20
1	1A	2233	U	O5'-P-OP2	-8.40	98.14	105.70
1	2A	1386	C	O5'-P-OP1	-8.40	98.14	105.70
1	2A	2237	G	C5-C6-O6	8.40	133.64	128.60
1	2A	1652	A	N1-C6-N6	-8.40	113.56	118.60
1	1A	1928	A	O5'-P-OP2	8.39	120.77	110.70
1	2A	463	G	C8-N9-C4	-8.39	103.04	106.40
1	1A	1997	G	OP1-P-OP2	-8.39	107.02	119.60
1	1A	780	G	C4-C5-N7	-8.39	107.44	110.80
1	2A	572	A	C8-N9-C4	-8.39	102.44	105.80
1	2A	793	A	O5'-P-OP2	-8.39	98.15	105.70
32	1a	299	G	C8-N9-C4	8.39	109.75	106.40
32	2a	1469	G	N1-C6-O6	8.39	124.93	119.90
1	2A	906	G	N3-C4-N9	-8.38	120.97	126.00
2	1B	89	G	N1-C6-O6	8.38	124.92	119.90
1	2A	193	U	N1-C2-O2	-8.38	116.94	122.80
1	1A	810	U	C5-C4-O4	-8.37	120.88	125.90
1	1A	2574	G	N1-C6-O6	-8.37	114.88	119.90
1	1A	593	G	O5'-P-OP2	-8.37	98.17	105.70
1	1A	655	A	C8-N9-C4	-8.37	102.45	105.80
1	1A	1187	G	C4-C5-N7	8.37	114.15	110.80
1	2A	436	C	N1-C2-O2	8.37	123.92	118.90
1	2A	1981	A	N1-C6-N6	8.36	123.62	118.60
1	2A	263	C	C6-N1-C2	8.36	123.64	120.30
1	2A	2427	C	C6-N1-C2	8.36	123.64	120.30
1	1A	1997	G	C8-N9-C4	-8.35	103.06	106.40
1	1A	2433	A	N1-C2-N3	8.35	133.48	129.30
1	2A	669	G	N3-C2-N2	-8.35	114.05	119.90
1	1A	1527	G	C5-C6-N1	-8.35	107.33	111.50
1	1A	1608	A	O5'-P-OP1	-8.34	98.19	105.70
1	1A	1144	G	OP1-P-OP2	-8.34	107.09	119.60
1	1A	446	G	C8-N9-C4	8.34	109.73	106.40
13	1R	8	ARG	NE-CZ-NH1	-8.34	116.13	120.30
1	2A	2061	G	O5'-P-OP2	-8.34	98.20	105.70
1	1A	2464	C	O5'-P-OP2	-8.33	98.20	105.70
32	2a	577	G	C2-N3-C4	-8.33	107.73	111.90
32	2a	299	G	C5-C6-O6	-8.33	123.60	128.60
32	2a	485	G	N3-C4-C5	-8.33	124.44	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1581	G	C8-N9-C4	-8.33	103.07	106.40
1	1A	2515	C	C6-N1-C2	8.32	123.63	120.30
1	2A	329	G	N3-C4-C5	-8.32	124.44	128.60
1	2A	1617	C	N1-C2-O2	8.32	123.89	118.90
32	2a	244	U	N1-C2-O2	8.31	128.62	122.80
1	1A	1786	A	N1-C2-N3	8.31	133.46	129.30
1	2A	209	C	C6-N1-C2	8.31	123.62	120.30
1	2A	1617	C	N3-C2-O2	-8.31	116.08	121.90
1	1A	401	A	N1-C2-N3	8.30	133.45	129.30
1	1A	2509	G	C4-C5-N7	8.30	114.12	110.80
2	1B	36	C	C6-N1-C2	8.30	123.62	120.30
1	2A	1639	U	N3-C2-O2	-8.30	116.39	122.20
1	2A	2822	G	C6-C5-N7	-8.30	125.42	130.40
1	2A	932	G	N3-C4-N9	-8.30	121.02	126.00
1	1A	2717	G	N1-C6-O6	8.30	124.88	119.90
1	1A	1972	A	C5-N7-C8	-8.29	99.75	103.90
1	1A	2623	G	C2-N3-C4	8.29	116.05	111.90
1	2A	988	A	N1-C6-N6	8.29	123.58	118.60
1	2A	2248	C	O5'-P-OP2	-8.29	98.24	105.70
1	1A	2848	G	O4'-C1'-N9	8.29	114.83	108.20
1	2A	229	A	C8-N9-C4	-8.29	102.48	105.80
1	2A	1992	G	C5-C6-N1	8.29	115.64	111.50
1	2A	2238	G	O5'-P-OP1	-8.29	98.24	105.70
1	1A	787	U	O5'-P-OP1	-8.29	98.24	105.70
1	2A	645	C	C2-N1-C1'	8.28	127.91	118.80
1	1A	563	G	N1-C6-O6	-8.28	114.93	119.90
32	2a	397	A	C8-N9-C4	-8.28	102.49	105.80
1	1A	27	G	O5'-P-OP1	-8.28	98.25	105.70
1	1A	1793	C	N1-C2-O2	-8.28	113.94	118.90
1	1A	1995	U	N1-C2-O2	-8.27	117.01	122.80
32	1a	576	G	C8-N9-C1'	-8.27	116.25	127.00
32	2a	346	G	C4-N9-C1'	8.27	137.25	126.50
1	1A	1340	U	N1-C2-O2	-8.27	117.01	122.80
1	2A	2060	A	O5'-P-OP1	-8.26	98.26	105.70
1	1A	177	G	N9-C4-C5	8.26	108.70	105.40
1	2A	377	C	C6-N1-C2	8.26	123.60	120.30
1	2A	558	G	O5'-P-OP2	-8.26	98.27	105.70
32	1a	354	G	O5'-P-OP2	-8.26	98.27	105.70
1	2A	1268	A	O5'-P-OP2	-8.26	98.27	105.70
1	2A	2515	C	O5'-P-OP2	-8.25	98.27	105.70
1	1A	2064	C	N3-C4-C5	-8.25	118.60	121.90
1	2A	1589	C	O5'-P-OP2	8.25	120.60	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2391	G	O4'-C1'-N9	8.25	114.80	108.20
1	1A	2070	G	C2-N3-C4	-8.24	107.78	111.90
1	2A	2415	G	N1-C6-O6	8.24	124.85	119.90
1	1A	1787	A	O5'-P-OP1	-8.24	98.28	105.70
1	2A	1307	A	C8-N9-C4	8.24	109.09	105.80
1	2A	452	G	N3-C4-C5	-8.24	124.48	128.60
1	1A	2823	A	C4-C5-C6	8.24	121.12	117.00
32	1a	343	U	C5-C4-O4	8.24	130.84	125.90
1	1A	2762	G	N3-C4-C5	8.23	132.72	128.60
2	1B	105	A	C8-N9-C4	8.23	109.09	105.80
1	1A	1653	G	N3-C4-N9	8.23	130.94	126.00
1	2A	1847	A	O4'-C1'-N9	8.23	114.79	108.20
2	2B	8	U	O5'-P-OP2	-8.23	98.29	105.70
1	1A	236	C	C2-N3-C4	-8.23	115.79	119.90
1	2A	1841	U	O5'-P-OP2	-8.23	98.30	105.70
1	2A	2319	G	C6-C5-N7	-8.23	125.47	130.40
1	1A	2246	G	C8-N9-C4	8.22	109.69	106.40
1	1A	2358	G	N1-C6-O6	8.22	124.83	119.90
32	1a	299	G	N9-C4-C5	-8.22	102.11	105.40
1	2A	1109	C	C6-N1-C2	-8.22	117.01	120.30
32	1a	841	U	C6-N1-C2	-8.22	116.07	121.00
1	1A	90	U	C5-C4-O4	8.22	130.83	125.90
1	1A	941	A	N9-C4-C5	8.22	109.09	105.80
1	1A	1254	A	C2-N3-C4	-8.22	106.49	110.60
1	1A	1477	A	O5'-P-OP2	-8.22	98.30	105.70
1	1A	2070	G	O5'-P-OP1	8.22	120.56	110.70
32	1a	427	U	N3-C2-O2	-8.22	116.45	122.20
1	2A	1797	C	C6-N1-C2	8.22	123.59	120.30
32	2a	1432	G	C5-C6-O6	8.21	133.53	128.60
1	1A	2390	U	N3-C4-O4	8.21	125.14	119.40
1	1A	2331	G	C2-N3-C4	-8.20	107.80	111.90
1	2A	959	A	C8-N9-C4	-8.20	102.52	105.80
1	2A	2062	A	N1-C6-N6	8.20	123.52	118.60
1	1A	2430	A	O5'-P-OP2	-8.20	98.32	105.70
1	1A	1187	G	C8-N9-C4	-8.19	103.12	106.40
2	1B	98	G	C5-C6-O6	-8.19	123.68	128.60
1	1A	463	G	C2-N3-C4	-8.19	107.81	111.90
1	1A	1132	A	OP1-P-OP2	8.19	131.89	119.60
1	2A	1607	C	N1-C2-O2	8.19	123.81	118.90
1	2A	1976	U	C6-N1-C2	-8.19	116.08	121.00
1	1A	330	A	C4-C5-N7	8.19	114.80	110.70
1	2A	451	C	C6-N1-C2	8.19	123.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	655	A	N7-C8-N9	8.19	117.89	113.80
32	1a	1431	C	C6-N1-C2	8.19	123.58	120.30
1	1A	2050	C	N1-C2-O2	-8.19	113.99	118.90
1	1A	195	A	P-O3'-C3'	8.18	129.52	119.70
1	2A	2609	U	C4-C5-C6	8.18	124.61	119.70
1	1A	1251	C	O5'-P-OP2	-8.18	98.34	105.70
1	2A	481	G	O5'-P-OP2	-8.18	98.34	105.70
1	2A	1264	G	N1-C6-O6	8.18	124.81	119.90
1	2A	2244	U	N1-C2-N3	8.18	119.81	114.90
1	1A	1753	G	N1-C6-O6	8.17	124.80	119.90
32	2a	651	C	C6-N1-C2	8.17	123.57	120.30
1	1A	529	A	C6-C5-N7	-8.17	126.58	132.30
1	1A	1653	G	C6-C5-N7	-8.17	125.50	130.40
1	2A	1109	C	N1-C2-O2	8.17	123.80	118.90
1	2A	1604	C	C6-N1-C2	-8.17	117.03	120.30
1	1A	1011	G	N7-C8-N9	-8.17	109.02	113.10
1	1A	2041	U	OP2-P-O3'	8.17	123.17	105.20
1	1A	2388	A	N1-C6-N6	-8.17	113.70	118.60
32	1a	558	G	C6-C5-N7	-8.17	125.50	130.40
1	1A	2848	G	C5-C6-O6	8.16	133.50	128.60
1	1A	513	A	C6-N1-C2	-8.16	113.70	118.60
1	1A	529	A	C5-C6-N1	8.16	121.78	117.70
1	2A	1325	G	N9-C4-C5	-8.16	102.14	105.40
1	2A	2886	G	C8-N9-C4	-8.15	103.14	106.40
1	1A	2041	U	C2-N3-C4	-8.15	122.11	127.00
32	2a	901	A	N1-C6-N6	8.15	123.49	118.60
1	1A	2483	C	N1-C2-O2	8.14	123.79	118.90
32	1a	804	U	O5'-P-OP2	-8.14	98.37	105.70
1	2A	818	G	N3-C4-N9	-8.14	121.11	126.00
1	2A	2714	G	C6-C5-N7	-8.14	125.51	130.40
1	1A	1566	A	C6-C5-N7	8.14	138.00	132.30
1	1A	2247	A	C2-N3-C4	-8.14	106.53	110.60
1	2A	271	A	C5-C6-N6	-8.14	117.19	123.70
32	1a	1442(A)	G	N1-C6-O6	8.14	124.78	119.90
1	2A	2078	C	C6-N1-C2	-8.13	117.05	120.30
1	1A	2509	G	C5-C6-N1	8.13	115.57	111.50
1	1A	2680	C	N3-C2-O2	8.13	127.59	121.90
1	1A	1780	A	OP1-P-OP2	8.13	131.79	119.60
1	1A	2613	U	N1-C2-O2	8.13	128.49	122.80
1	2A	387	U	O5'-P-OP2	-8.13	98.39	105.70
1	2A	2032	G	C6-N1-C2	-8.13	120.22	125.10
1	1A	956	G	C5-C6-N1	-8.12	107.44	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1342	A	N9-C4-C5	-8.12	102.55	105.80
32	2a	1079	G	C4-C5-N7	-8.13	107.55	110.80
1	1A	1801	G	C4-C5-N7	8.12	114.05	110.80
1	1A	585	G	O5'-P-OP2	8.12	120.44	110.70
1	2A	246	C	C6-N1-C2	8.12	123.55	120.30
1	1A	2598	A	O5'-P-OP1	-8.12	98.39	105.70
1	1A	1032	A	C8-N9-C4	8.12	109.05	105.80
1	1A	1801	G	C6-C5-N7	-8.12	125.53	130.40
1	2A	272(J)	C	C6-N1-C2	-8.12	117.05	120.30
1	1A	103	A	N1-C6-N6	8.11	123.47	118.60
1	1A	298	G	C5-N7-C8	8.11	108.35	104.30
1	1A	1824	G	C5-C6-O6	-8.11	123.73	128.60
1	1A	2721	A	O5'-P-OP2	8.11	120.43	110.70
1	1A	2663	G	C4-C5-N7	-8.11	107.56	110.80
1	2A	213	A	N1-C6-N6	-8.10	113.74	118.60
1	2A	463	G	N9-C4-C5	8.10	108.64	105.40
32	2a	748	C	N1-C2-O2	-8.10	114.04	118.90
32	2a	55	A	C8-N9-C4	-8.10	102.56	105.80
1	1A	448	U	N1-C2-N3	8.09	119.75	114.90
1	1A	733	G	C5-N7-C8	8.09	108.35	104.30
1	1A	1413	G	O5'-P-OP1	-8.09	98.42	105.70
1	2A	228	A	C5-N7-C8	-8.09	99.85	103.90
32	2a	264	U	C5-C4-O4	-8.09	121.05	125.90
1	1A	508	G	N3-C4-C5	8.09	132.65	128.60
1	1A	968	G	C5-C6-O6	8.09	133.46	128.60
1	2A	2291	U	O5'-P-OP2	-8.09	98.42	105.70
2	2B	59	A	C5-C6-N1	8.09	121.74	117.70
1	1A	821	A	O5'-P-OP2	-8.08	98.43	105.70
1	1A	2712(A)	A	C2-N3-C4	-8.08	106.56	110.60
1	2A	1312	U	C5-C4-O4	8.08	130.75	125.90
32	2a	1513	A	O5'-P-OP2	-8.08	98.43	105.70
1	1A	655	A	C5-N7-C8	-8.08	99.86	103.90
1	1A	1187	G	N3-C2-N2	8.08	125.55	119.90
1	1A	2474	C	C2-N1-C1'	8.07	127.68	118.80
2	1B	41	U	C5-C6-N1	-8.07	118.66	122.70
1	2A	1940	U	N3-C4-O4	8.07	125.05	119.40
1	1A	948	G	O5'-P-OP1	-8.07	98.44	105.70
1	1A	1344	G	C5-C6-N1	-8.07	107.47	111.50
1	2A	733	G	C8-N9-C4	8.07	109.63	106.40
1	1A	1430	C	O5'-P-OP2	-8.06	98.44	105.70
1	1A	2493	U	C5-C6-N1	-8.06	118.67	122.70
32	2a	535	A	N1-C6-N6	-8.06	113.76	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2499	C	C5-C6-N1	8.06	125.03	121.00
1	1A	54	G	C5-C6-N1	-8.05	107.47	111.50
1	1A	2245	U	C5-C6-N1	-8.05	118.67	122.70
1	1A	2249	U	C5-C4-O4	8.05	130.73	125.90
1	2A	670	A	N1-C6-N6	8.05	123.43	118.60
1	1A	139(A)	G	O5'-P-OP1	-8.04	98.46	105.70
1	1A	2616	C	N3-C4-C5	8.04	125.12	121.90
32	1a	1183	A	P-O3'-C3'	8.04	129.35	119.70
1	1A	2612	C	N1-C2-N3	-8.04	113.57	119.20
32	1a	1415	G	C5-C6-O6	-8.04	123.78	128.60
32	2a	1027	C	C5-C6-N1	8.04	125.02	121.00
32	1a	586	C	C6-N1-C2	8.03	123.51	120.30
1	1A	2242	G	N1-C6-O6	8.03	124.72	119.90
1	1A	559	G	N3-C2-N2	-8.03	114.28	119.90
1	1A	103	A	C4-C5-C6	8.03	121.01	117.00
1	1A	2030	A	C5-C6-N6	-8.03	117.28	123.70
1	1A	2817	G	N7-C8-N9	8.03	117.11	113.10
1	2A	1776	G	O5'-P-OP2	-8.03	98.47	105.70
1	1A	2578	G	C2-N3-C4	8.02	115.91	111.90
32	2a	1163	C	C6-N1-C2	-8.02	117.09	120.30
32	1a	1434	A	C8-N9-C4	8.02	109.01	105.80
1	1A	488	G	N9-C4-C5	8.02	108.61	105.40
1	1A	1452	A	N1-C6-N6	8.02	123.41	118.60
1	1A	2515	C	N3-C4-C5	8.02	125.11	121.90
2	1B	106	G	C8-N9-C4	8.02	109.61	106.40
1	1A	2502	G	O5'-P-OP1	-8.01	98.49	105.70
1	1A	1180	C	C6-N1-C2	8.01	123.50	120.30
1	1A	2068	U	C4-C5-C6	8.01	124.50	119.70
1	2A	252	G	C5-C6-O6	8.01	133.40	128.60
1	1A	1678	G	C5-C6-O6	-8.00	123.80	128.60
1	1A	2329	G	O5'-P-OP2	8.00	120.30	110.70
1	1A	1284	A	N9-C4-C5	-8.00	102.60	105.80
1	2A	2507	C	N3-C4-C5	-8.00	118.70	121.90
1	1A	942	G	C5-N7-C8	8.00	108.30	104.30
10	1O	23	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	2A	198	C	C2-N3-C4	-8.00	115.90	119.90
18	2W	23	LEU	CB-CG-CD2	-8.00	97.41	111.00
1	1A	779	U	O5'-P-OP2	7.99	120.29	110.70
1	1A	2443	C	N1-C2-N3	7.99	124.80	119.20
1	1A	2607	G	N3-C4-N9	-7.99	121.21	126.00
1	2A	315	G	O5'-P-OP2	-7.99	98.51	105.70
1	1A	582	G	C6-C5-N7	-7.99	125.61	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	892	A	C8-N9-C4	7.99	109.00	105.80
32	1a	529	G	N1-C6-O6	7.99	124.69	119.90
1	1A	715	G	N9-C4-C5	-7.98	102.21	105.40
1	1A	2237	G	O5'-P-OP2	-7.98	98.52	105.70
1	2A	452	G	N1-C2-N2	-7.98	109.02	116.20
32	1a	1319	A	N1-C6-N6	-7.98	113.81	118.60
1	1A	400	G	N1-C6-O6	7.98	124.69	119.90
1	2A	1991	U	O5'-P-OP2	-7.98	98.52	105.70
1	1A	2684	U	O5'-P-OP2	-7.97	98.52	105.70
10	1O	23	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	2A	391	G	C5-C6-O6	-7.97	123.81	128.60
1	1A	768	G	C2-N3-C4	-7.97	107.91	111.90
1	1A	838	C	N1-C2-O2	7.97	123.68	118.90
1	1A	2074	U	C6-N1-C2	-7.97	116.22	121.00
1	1A	615	G	C5-C6-N1	7.97	115.48	111.50
1	2A	778	G	O5'-P-OP1	-7.97	98.53	105.70
1	1A	73	A	C6-N1-C2	-7.97	113.82	118.60
1	1A	62	C	C5-C6-N1	-7.97	117.02	121.00
1	1A	1162	G	C5-C6-O6	7.97	133.38	128.60
1	1A	840	C	N3-C2-O2	7.96	127.47	121.90
1	1A	859	G	C8-N9-C4	7.96	109.58	106.40
1	1A	2487	G	C5-C6-O6	-7.96	123.82	128.60
1	2A	807	U	N1-C2-N3	7.96	119.68	114.90
1	1A	627	A	C8-N9-C4	7.96	108.98	105.80
1	1A	694	U	C5-C4-O4	7.96	130.68	125.90
1	2A	2319	G	C2-N3-C4	-7.96	107.92	111.90
1	1A	2553	G	N3-C4-C5	-7.96	124.62	128.60
32	1a	69	G	O5'-P-OP2	-7.96	98.54	105.70
1	2A	250	G	O5'-P-OP1	-7.96	98.54	105.70
1	2A	614	U	C5-C4-O4	7.96	130.68	125.90
3	2D	63	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	1A	1817	G	C5-C6-O6	7.96	133.37	128.60
1	2A	2375	G	C8-N9-C4	7.96	109.58	106.40
1	1A	1283	G	N1-C6-O6	-7.95	115.13	119.90
1	1A	2525	G	O5'-P-OP1	7.95	120.24	110.70
1	2A	2408	U	N1-C2-O2	7.95	128.37	122.80
32	1a	1529	G	N7-C8-N9	7.95	117.08	113.10
1	1A	972	G	O5'-P-OP2	-7.95	98.55	105.70
1	2A	2822	G	C4-C5-C6	7.95	123.57	118.80
1	2A	133	C	C5-C6-N1	-7.95	117.03	121.00
32	1a	23	C	C6-N1-C2	-7.94	117.12	120.30
32	1a	372	C	C6-N1-C2	7.94	123.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	308	G	C2-N3-C4	-7.94	107.93	111.90
32	1a	1495	U	C2-N3-C4	7.94	131.76	127.00
1	2A	566	U	C6-N1-C2	7.94	125.76	121.00
1	1A	599	G	N7-C8-N9	-7.94	109.13	113.10
1	2A	226	G	N9-C4-C5	7.94	108.58	105.40
1	2A	2822	G	C4-N9-C1'	7.94	136.82	126.50
1	1A	667	U	O5'-P-OP1	-7.93	98.56	105.70
1	1A	1954	G	N1-C6-O6	7.93	124.66	119.90
1	1A	683	C	N3-C4-C5	7.93	125.07	121.90
1	1A	2618	G	N9-C4-C5	7.93	108.57	105.40
1	2A	767	U	C5-C4-O4	7.92	130.65	125.90
1	2A	2111	C	C6-N1-C2	-7.92	117.13	120.30
1	2A	2057	A	O5'-P-OP2	-7.92	98.57	105.70
32	2a	1079	G	N9-C4-C5	7.92	108.57	105.40
1	1A	773	U	OP1-P-OP2	-7.92	107.72	119.60
1	1A	2511	U	C4-C5-C6	7.92	124.45	119.70
1	1A	1812	A	N1-C6-N6	-7.92	113.85	118.60
1	2A	1416	G	C8-N9-C4	7.91	109.56	106.40
1	2A	2319	G	C5-N7-C8	-7.91	100.34	104.30
32	2a	1137	C	C5-C6-N1	7.91	124.95	121.00
1	2A	2689	U	P-O3'-C3'	7.91	129.19	119.70
32	2a	291	C	C6-N1-C2	7.91	123.46	120.30
1	1A	385	C	C6-N1-C2	-7.91	117.14	120.30
1	1A	2852	G	C8-N9-C4	7.91	109.56	106.40
32	2a	495	A	N1-C6-N6	-7.90	113.86	118.60
1	1A	622	G	C6-C5-N7	-7.90	125.66	130.40
1	1A	1296	G	C8-N9-C4	7.90	109.56	106.40
1	2A	1678	G	C4-N9-C1'	7.89	136.76	126.50
1	1A	2780	G	C5-C6-O6	7.89	133.33	128.60
1	2A	2319	G	C4-N9-C1'	7.89	136.76	126.50
1	1A	383	U	N1-C2-O2	7.88	128.32	122.80
32	2a	903	G	C8-N9-C4	7.88	109.55	106.40
1	1A	2390	U	C2-N1-C1'	7.88	127.16	117.70
1	2A	988	A	C5-C6-N6	-7.88	117.40	123.70
1	2A	2773	C	N3-C4-C5	-7.87	118.75	121.90
1	1A	45	C	C6-N1-C2	7.87	123.45	120.30
1	1A	960	A	N1-C6-N6	7.87	123.32	118.60
1	1A	794	G	O5'-P-OP2	7.87	120.14	110.70
1	2A	1382	G	N1-C6-O6	7.87	124.62	119.90
1	2A	446	G	O5'-P-OP2	-7.87	98.62	105.70
1	2A	1320	C	C6-N1-C2	7.87	123.45	120.30
1	2A	228	A	C5-C6-N6	-7.86	117.41	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1231	G	O5'-P-OP2	7.86	120.14	110.70
1	1A	2511	U	C5-C6-N1	-7.86	118.77	122.70
1	1A	2691	C	N3-C4-C5	-7.86	118.76	121.90
1	2A	1858	G	N1-C6-O6	-7.86	115.19	119.90
32	2a	1252	A	N1-C6-N6	-7.86	113.89	118.60
1	1A	1643	G	N1-C6-O6	-7.86	115.19	119.90
1	2A	502	A	C8-N9-C4	7.86	108.94	105.80
2	1B	99	G	N7-C8-N9	-7.85	109.17	113.10
1	1A	1566	A	C5-C6-N6	7.85	129.98	123.70
1	1A	2627	G	C6-C5-N7	-7.85	125.69	130.40
1	1A	1762	A	N7-C8-N9	-7.85	109.88	113.80
1	1A	2179	C	C5-C6-N1	7.85	124.92	121.00
1	1A	2848	G	N1-C6-O6	-7.85	115.19	119.90
1	1A	2440	C	O5'-P-OP1	-7.84	98.64	105.70
1	2A	2556	C	C6-N1-C2	7.84	123.44	120.30
1	2A	55	G	C8-N9-C4	-7.84	103.26	106.40
32	1a	841	U	C5-C6-N1	7.84	126.62	122.70
1	1A	2767	C	C6-N1-C2	-7.84	117.17	120.30
1	2A	242	G	C8-N9-C4	7.84	109.53	106.40
1	1A	513	A	N3-C4-N9	7.83	133.67	127.40
1	1A	681	G	N3-C2-N2	-7.83	114.42	119.90
1	2A	12	U	C2-N1-C1'	7.83	127.10	117.70
1	1A	790	C	C5-C4-N4	-7.83	114.72	120.20
1	1A	1195	G	OP1-P-OP2	7.83	131.34	119.60
1	1A	1780	A	C8-N9-C4	-7.83	102.67	105.80
1	1A	2471	C	N3-C4-C5	-7.83	118.77	121.90
1	2A	2332	U	C5-C6-N1	-7.83	118.79	122.70
1	2A	2513	G	N1-C6-O6	7.83	124.60	119.90
32	2a	600	C	C6-N1-C2	7.83	123.43	120.30
32	2a	1026	G	C2-N3-C4	7.83	115.81	111.90
1	1A	512	G	O4'-C1'-N9	7.83	114.46	108.20
1	1A	807	U	C4-C5-C6	7.83	124.40	119.70
1	1A	1764	G	C8-N9-C4	-7.83	103.27	106.40
32	1a	1530	G	N9-C4-C5	-7.83	102.27	105.40
1	2A	664	C	C6-N1-C2	7.83	123.43	120.30
1	1A	662	G	N1-C2-N3	7.83	128.59	123.90
1	1A	1249	U	O5'-P-OP1	-7.83	98.66	105.70
1	2A	2444	G	O5'-P-OP1	-7.82	98.66	105.70
1	2A	2133	G	C4-N9-C1'	-7.82	116.33	126.50
1	2A	2394	C	C2-N3-C4	-7.82	115.99	119.90
2	1B	91	C	C6-N1-C2	7.82	123.43	120.30
32	2a	524	G	C8-N9-C4	-7.82	103.27	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1505	G	N9-C4-C5	7.82	108.53	105.40
1	2A	1990	C	C6-N1-C2	-7.82	117.17	120.30
1	1A	2699	C	N3-C2-O2	7.81	127.37	121.90
1	1A	391	G	N9-C4-C5	-7.81	102.28	105.40
1	1A	1823	G	N9-C4-C5	-7.81	102.28	105.40
2	1B	57	A	N9-C4-C5	-7.81	102.67	105.80
32	1a	1435	G	C5-C6-N1	-7.81	107.59	111.50
1	2A	1793	C	C6-N1-C2	7.81	123.42	120.30
1	1A	214	G	N9-C4-C5	-7.81	102.28	105.40
1	1A	752	A	N1-C6-N6	7.81	123.29	118.60
3	2D	242	ARG	NE-CZ-NH1	7.81	124.21	120.30
32	2a	841	U	C2-N1-C1'	7.81	127.07	117.70
1	1A	751	A	C8-N9-C4	-7.81	102.68	105.80
1	1A	2872	G	N1-C2-N3	7.81	128.59	123.90
1	2A	399	G	C4-C5-N7	7.81	113.92	110.80
1	2A	1284	A	O5'-P-OP2	-7.81	98.67	105.70
1	1A	1555	G	N1-C6-O6	7.80	124.58	119.90
1	1A	2179	C	C2-N1-C1'	7.80	127.38	118.80
1	2A	948	G	O5'-P-OP1	-7.80	98.68	105.70
32	1a	818	G	O5'-P-OP1	-7.80	98.68	105.70
1	1A	1372	U	C5-C4-O4	-7.80	121.22	125.90
1	1A	2430	A	N9-C4-C5	7.80	108.92	105.80
1	1A	126	A	N1-C2-N3	-7.80	125.40	129.30
1	1A	2088	G	N3-C4-C5	7.80	132.50	128.60
1	2A	995	C	C6-N1-C2	7.80	123.42	120.30
1	2A	1126	A	C8-N9-C4	7.80	108.92	105.80
1	1A	271	A	C8-N9-C4	7.79	108.92	105.80
1	1A	2220	G	N1-C6-O6	7.79	124.58	119.90
1	1A	2451	A	C5-N7-C8	-7.79	100.00	103.90
1	1A	2850	A	N1-C6-N6	7.79	123.28	118.60
32	1a	303	A	O5'-P-OP2	-7.79	98.69	105.70
1	2A	982	C	C5-C6-N1	7.79	124.89	121.00
1	1A	2510	C	C6-N1-C2	7.79	123.42	120.30
32	2a	1183	A	P-O3'-C3'	7.79	129.04	119.70
1	1A	1789	A	C2-N3-C4	-7.79	106.71	110.60
1	1A	2278	A	N1-C6-N6	7.78	123.27	118.60
32	1a	533	A	C4-C5-C6	7.78	120.89	117.00
1	2A	689	A	C2-N3-C4	7.78	114.49	110.60
1	1A	2252	G	C6-C5-N7	-7.78	125.73	130.40
32	1a	503	C	N3-C4-C5	-7.77	118.79	121.90
1	2A	738	G	C4-C5-N7	-7.77	107.69	110.80
1	1A	2032	G	N1-C6-O6	7.77	124.56	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2590	A	C4-C5-N7	7.77	114.58	110.70
1	2A	141	A	N1-C6-N6	7.77	123.26	118.60
1	2A	1321	A	N1-C2-N3	7.77	133.18	129.30
1	2A	2562	U	C4-C5-C6	7.77	124.36	119.70
1	1A	836	G	N1-C6-O6	-7.77	115.24	119.90
32	1a	750	G	O5'-P-OP1	-7.76	98.71	105.70
32	1a	284	G	C5-C6-N1	-7.76	107.62	111.50
1	1A	563	G	C5-C6-O6	7.76	133.26	128.60
32	2a	1523	G	O5'-P-OP2	-7.76	98.71	105.70
1	1A	2707	G	N7-C8-N9	-7.76	109.22	113.10
2	1B	50	G	O5'-P-OP2	-7.76	98.72	105.70
32	1a	1384	C	C6-N1-C2	-7.76	117.20	120.30
1	1A	2117	A	N1-C6-N6	-7.75	113.95	118.60
1	1A	2499	C	N3-C4-N4	7.75	123.43	118.00
32	1a	561	U	O5'-P-OP2	-7.75	98.72	105.70
1	2A	308	G	N1-C6-O6	7.75	124.55	119.90
1	1A	715	G	C8-N9-C1'	-7.75	116.92	127.00
1	1A	986	C	OP1-P-OP2	-7.75	107.97	119.60
1	1A	1777	U	C4-C5-C6	7.75	124.35	119.70
1	1A	2891	G	C5-C6-O6	-7.75	123.95	128.60
1	1A	981	A	C8-N9-C4	7.74	108.90	105.80
32	1a	656	C	C6-N1-C2	-7.74	117.20	120.30
1	1A	2026	C	C6-N1-C2	7.74	123.40	120.30
1	1A	1268	A	C6-N1-C2	-7.74	113.96	118.60
32	1a	521	G	N1-C6-O6	-7.74	115.26	119.90
1	1A	2230	G	O5'-P-OP2	7.74	119.98	110.70
1	1A	2483	C	C5-C4-N4	-7.74	114.78	120.20
32	1a	1397	C	C2-N1-C1'	7.74	127.31	118.80
1	1A	214	G	C8-N9-C4	7.73	109.49	106.40
1	1A	1482	G	O5'-P-OP2	-7.73	98.74	105.70
32	1a	299	G	C5-C6-O6	-7.73	123.96	128.60
1	2A	672	C	N1-C2-O2	7.73	123.54	118.90
1	1A	1212	G	C4-C5-N7	-7.73	107.71	110.80
1	1A	1969	A	O5'-P-OP1	-7.73	98.75	105.70
1	2A	1973	G	C5-C6-O6	7.73	133.24	128.60
1	2A	2280	G	C8-N9-C4	7.73	109.49	106.40
1	2A	2549	G	C8-N9-C4	7.73	109.49	106.40
1	1A	1196	C	C6-N1-C2	7.72	123.39	120.30
1	1A	481	G	N3-C4-C5	-7.72	124.74	128.60
1	1A	2371	G	C2-N3-C4	7.72	115.76	111.90
1	2A	2145	C	C5-C6-N1	7.72	124.86	121.00
1	1A	783	A	N7-C8-N9	7.72	117.66	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1406	U	C2-N3-C4	-7.72	122.37	127.00
1	2A	193	U	C4-C5-C6	7.72	124.33	119.70
1	1A	1165	U	C5-C4-O4	7.72	130.53	125.90
1	1A	739	G	O5'-P-OP2	7.72	119.96	110.70
1	2A	961	C	O5'-P-OP2	-7.72	98.75	105.70
1	1A	193	U	N1-C2-N3	7.71	119.53	114.90
1	1A	177	G	N1-C6-O6	-7.71	115.27	119.90
1	1A	1327	C	N3-C4-N4	7.71	123.40	118.00
1	1A	1800	C	N1-C2-N3	7.71	124.60	119.20
1	1A	2407	G	C4-C5-C6	7.71	123.43	118.80
1	1A	2314	C	C6-N1-C2	7.71	123.38	120.30
1	1A	259	G	C8-N9-C4	7.71	109.48	106.40
1	1A	2063	C	O5'-P-OP2	-7.71	98.76	105.70
1	1A	1266	G	N1-C6-O6	-7.71	115.28	119.90
1	2A	2656	U	C2-N1-C1'	7.70	126.94	117.70
1	1A	154(A)	C	N1-C2-O2	7.70	123.52	118.90
1	1A	2247	A	C4-C5-C6	7.70	120.85	117.00
1	2A	2313	C	C6-N1-C2	-7.70	117.22	120.30
1	1A	1212	G	C5-C6-O6	7.70	133.22	128.60
1	2A	327	G	N1-C6-O6	-7.70	115.28	119.90
1	2A	685	A	C2-N3-C4	7.70	114.45	110.60
1	1A	1992	G	C5-C6-O6	-7.70	123.98	128.60
1	2A	1662	C	O5'-P-OP2	-7.70	98.77	105.70
32	2a	721	G	C6-C5-N7	-7.70	125.78	130.40
32	2a	768	A	N1-C2-N3	7.70	133.15	129.30
1	1A	2002	G	N1-C6-O6	7.69	124.52	119.90
1	1A	1052	C	C6-N1-C2	-7.69	117.22	120.30
1	1A	1343	G	C4-N9-C1'	7.69	136.50	126.50
1	1A	2401	U	O5'-P-OP1	-7.69	98.78	105.70
1	1A	2607	G	C5-C6-N1	-7.69	107.65	111.50
1	1A	488	G	C5-C6-O6	7.69	133.21	128.60
32	1a	1076	C	N1-C2-O2	-7.69	114.29	118.90
1	2A	2319	G	N1-C2-N3	7.69	128.51	123.90
1	1A	40	C	N1-C2-O2	-7.69	114.29	118.90
1	1A	2483	C	C2-N1-C1'	7.69	127.26	118.80
1	2A	213	A	C4-C5-C6	-7.69	113.16	117.00
1	2A	2022	U	N3-C4-O4	7.69	124.78	119.40
1	1A	874	G	O5'-P-OP2	-7.69	98.78	105.70
32	2a	1378	C	N3-C4-C5	-7.69	118.83	121.90
1	1A	1801	G	C5-C6-O6	-7.68	123.99	128.60
1	2A	2822	G	N1-C6-O6	7.68	124.51	119.90
1	1A	2388	A	N9-C4-C5	7.68	108.87	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1021	A	C8-N9-C4	-7.68	102.73	105.80
32	2a	297	G	O5'-P-OP2	-7.68	98.79	105.70
1	1A	2024	G	C8-N9-C4	7.67	109.47	106.40
1	1A	781	A	C5-C6-N1	7.67	121.54	117.70
1	1A	2250	G	C5-C6-O6	7.67	133.20	128.60
1	2A	2755	C	C5-C4-N4	-7.67	114.83	120.20
32	2a	196	A	O5'-P-OP1	-7.67	98.80	105.70
1	1A	1203	G	C5-C6-O6	-7.67	124.00	128.60
1	1A	2252	G	C8-N9-C4	7.67	109.47	106.40
1	1A	2329	G	N7-C8-N9	-7.67	109.27	113.10
1	2A	451	C	N3-C4-C5	7.67	124.97	121.90
2	2B	5	C	C6-N1-C2	7.67	123.37	120.30
1	1A	1393	A	N1-C6-N6	-7.66	114.00	118.60
1	2A	1304	C	C6-N1-C2	7.66	123.37	120.30
1	2A	1439	A	O5'-P-OP1	-7.66	98.80	105.70
1	2A	312	G	O5'-P-OP1	-7.66	98.80	105.70
1	1A	2246	G	N9-C4-C5	-7.66	102.34	105.40
1	2A	2584	U	C6-N1-C2	-7.66	116.40	121.00
1	1A	1705	G	N1-C2-N3	7.66	128.50	123.90
1	2A	734	A	N1-C6-N6	7.66	123.19	118.60
1	2A	1006	C	O5'-P-OP1	-7.66	98.81	105.70
1	1A	2397	G	N7-C8-N9	7.66	116.93	113.10
1	1A	2608	G	N3-C2-N2	-7.66	114.54	119.90
1	2A	1820	U	C5-C4-O4	-7.65	121.31	125.90
1	2A	2240	C	N1-C2-O2	7.65	123.49	118.90
1	1A	45	C	N3-C4-C5	7.65	124.96	121.90
1	1A	491	G	O5'-P-OP1	-7.65	98.81	105.70
1	2A	1615	C	N3-C4-C5	-7.65	118.84	121.90
2	2B	115	G	N9-C4-C5	-7.65	102.34	105.40
1	1A	2371	G	C5-C6-N1	7.65	115.33	111.50
1	1A	224	G	N1-C6-O6	-7.65	115.31	119.90
1	2A	2556	C	C5-C4-N4	-7.65	114.85	120.20
2	1B	23	G	O5'-P-OP1	-7.65	98.82	105.70
1	2A	148	C	C5-C4-N4	-7.64	114.85	120.20
1	2A	746	A	O5'-P-OP2	7.64	119.87	110.70
1	2A	1815	A	N1-C2-N3	7.64	133.12	129.30
1	1A	1604	C	N1-C2-O2	-7.64	114.31	118.90
32	2a	78	G	C8-N9-C4	-7.64	103.34	106.40
1	1A	570	G	C8-N9-C4	-7.64	103.34	106.40
1	1A	1170	G	C8-N9-C4	-7.64	103.34	106.40
1	2A	2679	A	OP2-P-O3'	7.64	122.00	105.20
1	1A	235	U	C5-C6-N1	-7.64	118.88	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1847	A	C8-N9-C4	-7.64	102.75	105.80
1	1A	2499	C	C6-N1-C2	-7.64	117.25	120.30
32	2a	508	C	C6-N1-C1'	-7.64	111.64	120.80
1	1A	2650	U	C6-N1-C2	7.63	125.58	121.00
1	1A	2662	A	N7-C8-N9	7.63	117.62	113.80
1	1A	713	G	C5-C6-N1	-7.63	107.69	111.50
1	2A	1109	C	N3-C2-O2	-7.63	116.56	121.90
1	2A	1123	C	C6-N1-C2	7.63	123.35	120.30
1	1A	1407	C	N3-C4-C5	-7.63	118.85	121.90
1	1A	259	G	C5-C6-O6	-7.62	124.03	128.60
1	1A	335	C	C2-N3-C4	7.62	123.71	119.90
1	1A	655	A	C2-N3-C4	-7.62	106.79	110.60
1	2A	2319	G	C4-C5-N7	7.62	113.85	110.80
1	1A	205	G	O5'-P-OP2	-7.62	98.84	105.70
1	1A	1153	C	C6-N1-C2	-7.62	117.25	120.30
1	1A	1455	G	C4-C5-N7	7.62	113.85	110.80
1	2A	831	G	O5'-P-OP1	-7.62	98.84	105.70
1	2A	2267	A	N1-C6-N6	7.62	123.17	118.60
1	2A	2378	A	C6-C5-N7	-7.62	126.97	132.30
32	1a	266	G	P-O3'-C3'	7.62	128.84	119.70
1	1A	624	C	C6-N1-C2	7.62	123.35	120.30
1	1A	944	G	N7-C8-N9	7.62	116.91	113.10
1	1A	684	G	N1-C6-O6	-7.62	115.33	119.90
1	2A	226	G	C2-N3-C4	7.62	115.71	111.90
1	2A	2427	C	N3-C2-O2	7.62	127.23	121.90
1	1A	1888	G	C5-C6-O6	-7.61	124.03	128.60
1	2A	580	C	N3-C4-C5	-7.61	118.86	121.90
1	2A	2331	G	C8-N9-C4	7.61	109.44	106.40
1	1A	2130	U	C5-C6-N1	7.61	126.50	122.70
1	1A	1036	G	C8-N9-C4	7.61	109.44	106.40
1	1A	1323	U	N1-C2-N3	7.61	119.47	114.90
1	1A	1832	C	O5'-P-OP2	-7.61	98.85	105.70
1	1A	2717	G	C5-C6-O6	-7.61	124.03	128.60
1	1A	267	C	C6-N1-C2	7.61	123.34	120.30
1	2A	2046	G	C8-N9-C4	7.61	109.44	106.40
1	1A	1753	G	C5-N7-C8	-7.60	100.50	104.30
32	2a	343	U	C6-N1-C1'	7.60	131.84	121.20
1	1A	2247	A	N1-C2-N3	7.60	133.10	129.30
1	1A	729	G	C4-C5-N7	7.60	113.84	110.80
1	1A	1300	U	O5'-P-OP2	-7.60	98.86	105.70
1	2A	906	G	C8-N9-C1'	7.60	136.88	127.00
1	1A	2499	C	C2-N3-C4	7.60	123.70	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	942	G	C4-C5-N7	-7.59	107.76	110.80
1	1A	1789	A	C8-N9-C4	7.59	108.84	105.80
1	1A	2639	A	N1-C6-N6	7.59	123.16	118.60
32	1a	1505	G	C6-C5-N7	7.59	134.96	130.40
1	2A	1897	G	C8-N9-C4	7.59	109.44	106.40
1	2A	2468	G	C5-C6-N1	-7.59	107.70	111.50
1	1A	766	C	C6-N1-C2	7.59	123.34	120.30
1	1A	622	G	C8-N9-C1'	-7.59	117.13	127.00
1	1A	2431	U	C6-N1-C2	7.59	125.55	121.00
1	2A	148	C	N3-C2-O2	7.59	127.21	121.90
1	1A	1064	C	N1-C2-O2	7.58	123.45	118.90
1	1A	1780	A	N1-C2-N3	7.58	133.09	129.30
1	1A	1721	G	C4-C5-N7	7.58	113.83	110.80
1	1A	1756	G	C5-C6-O6	7.58	133.15	128.60
1	1A	2250	G	N3-C4-N9	-7.58	121.45	126.00
1	1A	465	G	N3-C4-N9	7.58	130.55	126.00
1	1A	951	C	N3-C4-C5	-7.58	118.87	121.90
1	2A	2032	G	N7-C8-N9	-7.58	109.31	113.10
1	1A	1676	A	C2-N3-C4	-7.58	106.81	110.60
1	1A	2485	G	N7-C8-N9	-7.58	109.31	113.10
32	1a	576	G	C4-C5-C6	7.58	123.35	118.80
1	2A	672	C	N3-C2-O2	-7.58	116.59	121.90
32	2a	721	G	N1-C6-O6	7.58	124.45	119.90
1	2A	2238	G	C8-N9-C4	-7.58	103.37	106.40
1	1A	2853	C	O5'-P-OP1	7.58	119.79	110.70
1	1A	2371	G	C8-N9-C4	7.57	109.43	106.40
1	2A	383	U	C2-N3-C4	7.57	131.54	127.00
1	1A	725	G	C4-N9-C1'	7.57	136.34	126.50
1	1A	2356	C	N1-C2-O2	-7.57	114.36	118.90
1	2A	2144	U	C5-C6-N1	7.57	126.48	122.70
1	1A	1187	G	N1-C6-O6	-7.57	115.36	119.90
1	1A	2863	C	C6-N1-C2	7.57	123.33	120.30
1	2A	329	G	O5'-P-OP2	7.57	119.78	110.70
1	1A	773	U	C5-C6-N1	-7.57	118.92	122.70
1	1A	104	U	N1-C2-O2	-7.57	117.50	122.80
1	1A	2040	C	N1-C2-N3	-7.57	113.90	119.20
1	1A	1466	G	N3-C2-N2	-7.56	114.61	119.90
1	2A	783	A	O5'-P-OP2	-7.56	98.89	105.70
32	2a	1278	U	N1-C2-O2	7.56	128.09	122.80
1	1A	607	U	C5-C6-N1	-7.56	118.92	122.70
1	1A	838	C	N3-C2-O2	-7.56	116.61	121.90
1	1A	582	G	C2-N3-C4	-7.56	108.12	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	784	A	P-O3'-C3'	7.56	128.77	119.70
1	2A	948	G	N3-C4-C5	7.56	132.38	128.60
1	1A	330	A	N1-C2-N3	7.56	133.08	129.30
1	1A	2464	C	C6-N1-C2	7.55	123.32	120.30
1	1A	1954	G	C5-C6-O6	-7.55	124.07	128.60
1	1A	1410	G	N3-C4-C5	7.55	132.38	128.60
1	1A	712	G	C5-C6-O6	-7.55	124.07	128.60
1	1A	738	G	OP2-P-O3'	7.55	121.80	105.20
1	2A	1644	C	N1-C2-O2	7.54	123.43	118.90
1	1A	1772	G	C8-N9-C4	7.54	109.42	106.40
1	2A	733	G	N9-C4-C5	-7.54	102.38	105.40
1	2A	2446	G	O5'-P-OP2	-7.54	98.91	105.70
32	2a	117	G	O5'-P-OP2	-7.54	98.91	105.70
1	1A	1409	C	C6-N1-C2	7.54	123.32	120.30
32	1a	1480	G	C2-N3-C4	-7.54	108.13	111.90
1	2A	1671	U	C5-C6-N1	-7.54	118.93	122.70
1	1A	461	C	N3-C4-C5	-7.54	118.88	121.90
1	1A	2437	U	N1-C2-O2	-7.54	117.52	122.80
32	1a	1442(A)	G	C6-C5-N7	-7.54	125.88	130.40
1	1A	1047	G	C4-N9-C1'	7.54	136.30	126.50
1	2A	386	G	N3-C2-N2	-7.54	114.62	119.90
1	2A	808	G	N1-C2-N3	-7.54	119.38	123.90
1	1A	829	A	N7-C8-N9	-7.54	110.03	113.80
1	2A	734	A	C2-N3-C4	-7.54	106.83	110.60
1	2A	2246	G	N1-C6-O6	7.53	124.42	119.90
1	1A	1429	G	O5'-P-OP2	-7.53	98.92	105.70
1	2A	315	G	O5'-P-OP1	7.53	119.74	110.70
1	1A	310	A	OP1-P-O3'	7.53	121.77	105.20
1	2A	2092	U	C5-C4-O4	-7.53	121.38	125.90
1	1A	246	C	N1-C2-O2	-7.53	114.38	118.90
1	1A	645	C	N1-C2-O2	7.53	123.42	118.90
1	2A	128	C	O5'-P-OP2	-7.53	98.92	105.70
1	2A	465	G	N3-C4-N9	7.53	130.52	126.00
1	1A	2424	C	C6-N1-C2	7.53	123.31	120.30
1	1A	2693	A	N1-C6-N6	7.53	123.12	118.60
1	2A	133	C	C4-C5-C6	7.53	121.16	117.40
1	2A	2591	C	N1-C2-O2	-7.53	114.38	118.90
1	1A	1527	G	C4-C5-C6	7.52	123.31	118.80
1	1A	2682	U	O5'-P-OP2	-7.52	98.93	105.70
1	1A	194	G	C8-N9-C4	7.52	109.41	106.40
2	1B	98	G	C8-N9-C4	7.52	109.41	106.40
1	1A	578	A	N1-C6-N6	-7.52	114.09	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1510	U	C5-C6-N1	-7.52	118.94	122.70
1	2A	1900	A	N1-C6-N6	7.52	123.11	118.60
1	2A	1108	U	N3-C4-O4	7.52	124.66	119.40
32	2a	1003	G	N3-C4-C5	-7.52	124.84	128.60
32	2a	1436	U	C2-N3-C4	-7.52	122.49	127.00
1	2A	1657	C	OP2-P-O3'	7.51	121.73	105.20
1	1A	1992	G	C8-N9-C4	7.51	109.41	106.40
1	1A	2294	C	N1-C2-O2	7.51	123.41	118.90
1	2A	1338	G	OP1-P-OP2	-7.51	108.33	119.60
32	2a	1495	U	C2-N1-C1'	7.51	126.72	117.70
32	1a	297	G	N1-C6-O6	7.51	124.41	119.90
1	2A	2733	A	C8-N9-C4	-7.51	102.80	105.80
1	1A	2442	C	C6-N1-C2	7.51	123.30	120.30
1	2A	720	C	C6-N1-C2	7.51	123.30	120.30
1	1A	1975	G	C5-C6-O6	-7.50	124.10	128.60
1	2A	645	C	C5-C6-N1	7.50	124.75	121.00
1	2A	1065	U	O4'-C1'-N1	7.50	114.20	108.20
1	1A	341	G	N1-C6-O6	-7.50	115.40	119.90
1	2A	808	G	C2-N3-C4	7.50	115.65	111.90
1	2A	1210	A	C8-N9-C4	-7.50	102.80	105.80
1	1A	432	A	N1-C6-N6	7.50	123.10	118.60
1	2A	906	G	C5-C6-O6	7.50	133.10	128.60
1	2A	2288	A	N1-C6-N6	7.50	123.10	118.60
1	1A	983	A	C8-N9-C4	7.50	108.80	105.80
32	2a	730	G	C4-C5-N7	-7.50	107.80	110.80
32	1a	904	C	C6-N1-C2	7.49	123.30	120.30
1	2A	909	A	N1-C6-N6	-7.49	114.10	118.60
2	1B	113	G	O5'-P-OP1	-7.49	98.96	105.70
1	2A	1066	U	C5-C6-N1	7.49	126.45	122.70
1	2A	1293	C	N1-C2-O2	-7.49	114.41	118.90
1	2A	1300	U	O5'-P-OP2	-7.49	98.96	105.70
2	2B	115	G	N3-C4-C5	7.49	132.34	128.60
1	1A	1339	G	C8-N9-C4	-7.49	103.41	106.40
32	2a	49	U	C5-C6-N1	-7.49	118.96	122.70
1	1A	2071	A	N1-C2-N3	7.49	133.04	129.30
1	1A	2582	G	C8-N9-C4	-7.49	103.41	106.40
2	1B	75	G	C5-C6-O6	-7.49	124.11	128.60
1	1A	519	U	O5'-P-OP2	-7.49	98.96	105.70
1	1A	1248	G	C5-C6-O6	-7.49	124.11	128.60
1	1A	1343	G	C6-C5-N7	-7.49	125.91	130.40
32	1a	1465	C	C2-N3-C4	-7.49	116.16	119.90
1	2A	827	U	C6-N1-C2	7.48	125.49	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	729	G	C6-C5-N7	-7.48	125.91	130.40
2	1B	39	A	C8-N9-C4	-7.48	102.81	105.80
1	2A	982	C	N3-C4-C5	-7.48	118.91	121.90
1	2A	670	A	N9-C4-C5	-7.48	102.81	105.80
1	2A	2458	G	N1-C6-O6	-7.48	115.41	119.90
1	1A	2850	A	N9-C4-C5	-7.48	102.81	105.80
1	1A	1300	U	N1-C2-N3	7.48	119.39	114.90
32	1a	801	U	N3-C4-C5	7.48	119.08	114.60
32	2a	1028	C	C5-C6-N1	7.48	124.74	121.00
1	1A	1304	C	C6-N1-C2	7.47	123.29	120.30
1	1A	2030	A	N1-C6-N6	7.47	123.08	118.60
1	2A	2031	A	N1-C6-N6	7.47	123.08	118.60
1	1A	1327	C	N3-C2-O2	7.47	127.13	121.90
1	1A	2164	C	C6-N1-C2	-7.47	117.31	120.30
32	1a	226	G	N9-C4-C5	-7.47	102.41	105.40
1	2A	2609	U	N1-C2-N3	7.47	119.38	114.90
1	1A	742	G	N1-C6-O6	7.47	124.38	119.90
1	1A	2650	U	C5-C6-N1	-7.47	118.97	122.70
1	2A	1846	G	O5'-P-OP2	-7.47	98.98	105.70
1	1A	250	G	C8-N9-C4	-7.46	103.41	106.40
1	1A	1966	A	C8-N9-C4	7.46	108.79	105.80
1	2A	391	G	C6-C5-N7	-7.46	125.92	130.40
1	2A	2585	U	C2-N1-C1'	7.46	126.66	117.70
1	1A	2829	C	N3-C4-N4	7.46	123.22	118.00
32	1a	1442(A)	G	C4-C5-N7	7.46	113.78	110.80
1	1A	1047	G	C5-C6-N1	7.46	115.23	111.50
1	1A	428	A	C4-C5-C6	7.46	120.73	117.00
1	1A	1253	A	C4-C5-C6	7.46	120.73	117.00
1	2A	827	U	N1-C2-O2	-7.46	117.58	122.80
32	2a	826	C	C5-C6-N1	-7.46	117.27	121.00
1	1A	724	U	C5-C4-O4	7.45	130.37	125.90
32	1a	1113	C	C6-N1-C2	-7.45	117.32	120.30
1	2A	606	U	C5-C4-O4	7.45	130.37	125.90
1	2A	1940	U	C5-C6-N1	7.45	126.43	122.70
32	2a	1478	C	C6-N1-C2	-7.45	117.32	120.30
1	2A	1325	G	N1-C2-N2	-7.45	109.49	116.20
1	1A	792	G	N1-C2-N2	-7.45	109.49	116.20
32	1a	1192	C	C6-N1-C2	-7.45	117.32	120.30
1	1A	844	C	C6-N1-C2	7.45	123.28	120.30
1	1A	1340	U	C4-C5-C6	7.45	124.17	119.70
32	2a	776	G	C5-C6-N1	-7.45	107.78	111.50
1	1A	1231	G	C8-N9-C4	-7.44	103.42	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2272	U	O5'-P-OP2	-7.44	99.00	105.70
32	1a	784	C	C5-C6-N1	-7.44	117.28	121.00
32	2a	568	G	O5'-P-OP1	-7.44	99.00	105.70
1	1A	259	G	N9-C4-C5	-7.44	102.42	105.40
1	1A	1632	A	C4-C5-C6	7.44	120.72	117.00
1	1A	1758	G	C8-N9-C4	-7.44	103.42	106.40
32	1a	533	A	N3-C4-N9	7.44	133.35	127.40
32	2a	508	C	C2-N1-C1'	7.44	126.98	118.80
1	1A	508	G	OP1-P-OP2	7.44	130.76	119.60
1	2A	1992	G	C5-C6-O6	-7.44	124.14	128.60
1	1A	2564	A	N1-C6-N6	7.44	123.06	118.60
32	1a	1523	G	C8-N9-C4	-7.43	103.43	106.40
1	1A	2429	G	C8-N9-C4	-7.43	103.43	106.40
32	1a	576	G	N3-C4-N9	7.43	130.46	126.00
32	1a	766	A	C8-N9-C4	7.43	108.77	105.80
1	2A	570	G	N3-C2-N2	7.43	125.10	119.90
1	1A	573	G	C8-N9-C4	-7.43	103.43	106.40
1	1A	2056	G	N3-C4-N9	7.43	130.46	126.00
1	2A	145	G	N7-C8-N9	-7.43	109.39	113.10
1	1A	2789	C	N3-C4-N4	-7.43	112.80	118.00
1	1A	1645	G	C5-C6-N1	7.43	115.21	111.50
1	2A	482	A	N1-C6-N6	7.43	123.06	118.60
32	2a	728	A	C6-C5-N7	-7.43	127.10	132.30
32	2a	1019	C	C6-N1-C2	-7.43	117.33	120.30
1	1A	1678	G	N1-C2-N3	7.42	128.35	123.90
1	1A	2538	C	N3-C4-C5	7.42	124.87	121.90
1	1A	2042	A	C8-N9-C4	7.42	108.77	105.80
1	1A	856	C	C5-C6-N1	7.42	124.71	121.00
32	1a	738	C	C6-N1-C2	-7.42	117.33	120.30
1	2A	1638	C	N1-C2-O2	-7.42	114.45	118.90
1	1A	713	G	N3-C4-C5	7.41	132.31	128.60
1	1A	806	C	C5-C6-N1	7.41	124.71	121.00
1	1A	2319	G	N9-C4-C5	-7.41	102.44	105.40
32	1a	1442	G	N3-C4-N9	7.41	130.45	126.00
1	1A	2555	U	N1-C2-O2	-7.41	117.61	122.80
3	1D	52	ARG	NE-CZ-NH1	-7.41	116.59	120.30
1	1A	844	C	C5-C6-N1	-7.41	117.30	121.00
1	1A	2848	G	N9-C4-C5	7.41	108.36	105.40
1	1A	810	U	N3-C4-O4	7.41	124.58	119.40
1	1A	2438	U	C5-C6-N1	-7.41	119.00	122.70
1	2A	189	G	N7-C8-N9	-7.41	109.40	113.10
1	2A	2018	G	C4-C5-N7	7.40	113.76	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	204	A	C6-N1-C2	-7.40	114.16	118.60
1	1A	462	C	C6-N1-C2	7.40	123.26	120.30
1	1A	1131	G	C5-C6-O6	7.40	133.04	128.60
2	2B	62	C	N3-C4-C5	-7.40	118.94	121.90
1	1A	2280	G	N1-C6-O6	-7.40	115.46	119.90
32	1a	1467	G	C5-C6-O6	7.40	133.04	128.60
32	2a	357	G	N3-C2-N2	-7.40	114.72	119.90
1	1A	2422	A	C5-C6-N1	-7.40	114.00	117.70
32	1a	801	U	C5-C6-N1	-7.40	119.00	122.70
1	2A	584	C	N3-C2-O2	7.40	127.08	121.90
1	1A	195	A	O5'-P-OP1	7.39	119.57	110.70
1	1A	1019	U	O5'-P-OP2	-7.39	99.05	105.70
1	1A	2715	C	C2-N3-C4	-7.39	116.20	119.90
1	1A	2829	C	N3-C2-O2	7.39	127.07	121.90
32	2a	1003	G	N7-C8-N9	7.39	116.80	113.10
1	2A	179	G	C8-N9-C4	7.39	109.36	106.40
1	1A	693	C	C2-N3-C4	-7.39	116.20	119.90
1	1A	1304	C	N3-C4-N4	-7.39	112.83	118.00
1	1A	2585	U	N3-C4-C5	7.39	119.03	114.60
1	1A	255	A	C6-N1-C2	-7.39	114.17	118.60
1	1A	2437	U	N3-C4-O4	7.39	124.57	119.40
32	1a	442	C	C5-C6-N1	7.39	124.69	121.00
1	1A	676	A	OP1-P-OP2	7.38	130.68	119.60
1	2A	2714	G	N9-C4-C5	-7.38	102.45	105.40
1	1A	806	C	N1-C2-O2	7.38	123.33	118.90
1	1A	1020	A	C8-N9-C4	-7.38	102.85	105.80
2	1B	69	G	O5'-P-OP2	-7.38	99.06	105.70
1	2A	1611	C	O5'-P-OP2	7.38	119.56	110.70
32	2a	769	G	C5-C6-N1	-7.38	107.81	111.50
1	1A	345	A	C8-N9-C4	-7.38	102.85	105.80
1	1A	2820	A	N9-C4-C5	-7.38	102.85	105.80
1	2A	2453	A	C5-N7-C8	7.38	107.59	103.90
1	2A	2451	A	C5-N7-C8	-7.38	100.21	103.90
1	2A	1817	G	N1-C6-O6	-7.37	115.47	119.90
4	2E	144	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	1A	782	A	C5-C6-N6	-7.37	117.80	123.70
1	2A	450	G	N1-C6-O6	-7.37	115.48	119.90
1	1A	371	A	N1-C6-N6	7.37	123.02	118.60
1	1A	944	G	C8-N9-C4	-7.36	103.45	106.40
1	1A	1758	G	N9-C4-C5	7.36	108.34	105.40
1	1A	1186	G	N7-C8-N9	-7.36	109.42	113.10
1	2A	1280	G	N7-C8-N9	-7.36	109.42	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2474	C	C6-N1-C1'	-7.36	111.97	120.80
1	1A	1765	C	O5'-P-OP2	-7.36	99.08	105.70
1	2A	303	U	O5'-P-OP2	-7.36	99.08	105.70
1	2A	690	G	N1-C6-O6	7.36	124.31	119.90
32	2a	893	C	C6-N1-C1'	-7.36	111.97	120.80
1	1A	366	C	N1-C2-O2	-7.36	114.49	118.90
32	1a	770	C	O5'-P-OP1	7.36	119.53	110.70
1	2A	2019	A	C5-N7-C8	7.36	107.58	103.90
32	2a	564	C	C6-N1-C2	7.36	123.24	120.30
32	2a	907	A	O5'-P-OP1	7.36	119.53	110.70
1	1A	1753	G	C5-C6-O6	-7.35	124.19	128.60
1	1A	465	G	N3-C4-C5	-7.35	124.92	128.60
1	1A	1665	A	O5'-P-OP1	-7.35	99.08	105.70
1	2A	687	C	C2-N3-C4	-7.35	116.23	119.90
32	1a	600	C	C6-N1-C2	7.35	123.24	120.30
1	1A	975(A)	G	N3-C2-N2	-7.34	114.76	119.90
1	1A	1644	C	C2-N3-C4	-7.34	116.23	119.90
32	1a	1246	C	C6-N1-C2	-7.34	117.36	120.30
1	2A	512	G	O4'-C1'-N9	7.34	114.08	108.20
32	2a	346	G	C8-N9-C1'	-7.34	117.45	127.00
1	1A	20	C	C2-N3-C4	-7.34	116.23	119.90
1	1A	711	G	N1-C6-O6	7.34	124.30	119.90
1	2A	2496	C	O5'-P-OP1	-7.34	99.09	105.70
32	1a	576	G	N3-C4-C5	-7.34	124.93	128.60
1	2A	48	G	C5-C6-N1	-7.34	107.83	111.50
1	2A	391	G	N1-C6-O6	7.34	124.30	119.90
1	2A	645	C	C6-N1-C2	-7.34	117.36	120.30
32	2a	163	C	C6-N1-C2	-7.34	117.36	120.30
1	2A	1210	A	P-O3'-C3'	7.34	128.50	119.70
1	2A	2439	A	N1-C6-N6	7.34	123.00	118.60
1	1A	391	G	C8-N9-C1'	-7.34	117.46	127.00
1	1A	826	U	N1-C2-O2	-7.34	117.66	122.80
1	2A	2144	U	C6-N1-C2	-7.34	116.60	121.00
1	2A	2454	G	O5'-P-OP1	-7.34	99.10	105.70
2	2B	6	C	C5-C6-N1	-7.34	117.33	121.00
1	2A	912	C	C6-N1-C2	-7.33	117.37	120.30
1	1A	828	U	C5-C4-O4	-7.33	121.50	125.90
1	1A	2618	G	N3-C4-C5	-7.33	124.93	128.60
1	2A	2488	A	N1-C6-N6	7.33	123.00	118.60
1	2A	2566	A	O5'-P-OP2	-7.33	99.10	105.70
1	1A	1323	U	C6-N1-C2	-7.33	116.60	121.00
1	1A	2491	U	C4-C5-C6	-7.33	115.30	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	467	G	C8-N9-C4	7.33	109.33	106.40
1	1A	2054	A	OP1-P-O3'	-7.33	89.08	105.20
1	1A	2476	A	O5'-P-OP2	-7.33	99.10	105.70
32	1a	175	C	C6-N1-C2	-7.33	117.37	120.30
1	1A	826	U	C5-C6-N1	-7.33	119.04	122.70
1	2A	1858	G	C5-C6-O6	7.33	133.00	128.60
1	1A	2662	A	C4-C5-C6	7.32	120.66	117.00
32	1a	863	U	C2-N1-C1'	-7.32	108.91	117.70
1	2A	1696	G	O5'-P-OP2	-7.32	99.11	105.70
1	1A	1480	G	O5'-P-OP2	7.32	119.49	110.70
32	2a	1418	A	N1-C6-N6	7.32	122.99	118.60
1	1A	1363	C	C5-C4-N4	7.32	125.32	120.20
32	1a	911	U	N1-C2-N3	7.32	119.29	114.90
1	1A	2369	A	C8-N9-C4	-7.32	102.87	105.80
1	1A	2857	G	N1-C6-O6	-7.32	115.51	119.90
1	1A	398	G	C8-N9-C4	7.31	109.33	106.40
1	1A	940	G	C8-N9-C4	-7.31	103.47	106.40
1	1A	2044	C	C6-N1-C2	-7.31	117.38	120.30
1	1A	2448	A	O5'-P-OP2	7.31	119.47	110.70
1	1A	2641	G	C8-N9-C4	-7.31	103.47	106.40
1	2A	2319	G	N1-C2-N2	-7.31	109.62	116.20
32	2a	869	G	O5'-P-OP1	-7.31	99.12	105.70
1	1A	201	C	C6-N1-C2	7.31	123.22	120.30
1	1A	1847	A	C4-N9-C1'	7.31	139.46	126.30
1	2A	1834	U	N3-C2-O2	-7.31	117.08	122.20
32	1a	321	A	C8-N9-C4	7.31	108.72	105.80
1	2A	800	A	C2-N3-C4	-7.31	106.94	110.60
1	2A	1108	U	C5-C6-N1	7.31	126.36	122.70
1	1A	83	G	C8-N9-C4	7.31	109.32	106.40
1	1A	2249	U	N1-C2-O2	7.31	127.92	122.80
1	2A	463	G	C5-C6-O6	7.31	132.99	128.60
1	2A	2739	U	N3-C2-O2	-7.31	117.08	122.20
1	1A	1770	G	C8-N9-C4	7.30	109.32	106.40
1	2A	207	A	N1-C2-N3	7.30	132.95	129.30
1	1A	2041	U	N3-C2-O2	7.30	127.31	122.20
1	1A	2596	U	O5'-P-OP1	-7.30	99.13	105.70
2	2B	24	G	N3-C4-N9	7.30	130.38	126.00
1	2A	1265	A	OP1-P-OP2	7.30	130.55	119.60
1	2A	2031	A	C5-C6-N6	-7.30	117.86	123.70
32	2a	581	G	N1-C6-O6	7.30	124.28	119.90
1	2A	1254	A	N1-C2-N3	7.30	132.95	129.30
1	2A	2005	A	C5-C6-N1	7.30	121.35	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	577	G	N3-C4-C5	7.30	132.25	128.60
1	1A	1224	C	C6-N1-C2	7.30	123.22	120.30
1	2A	2319	G	N7-C8-N9	7.30	116.75	113.10
1	1A	1290	C	C6-N1-C2	-7.29	117.38	120.30
1	2A	1374	G	C6-C5-N7	-7.29	126.02	130.40
1	1A	2627	G	N1-C6-O6	7.29	124.28	119.90
32	1a	818	G	C4-C5-N7	-7.29	107.88	110.80
1	2A	1815	A	C6-N1-C2	-7.29	114.22	118.60
1	1A	622	G	N9-C4-C5	-7.29	102.48	105.40
1	1A	1612	C	C5-C4-N4	-7.29	115.10	120.20
1	2A	1653	G	C8-N9-C1'	-7.29	117.52	127.00
1	1A	693	C	N3-C4-C5	7.29	124.82	121.90
32	1a	481	G	N9-C4-C5	-7.29	102.48	105.40
32	1a	1228	C	C6-N1-C2	-7.29	117.39	120.30
1	2A	2394	C	C5-C6-N1	-7.29	117.36	121.00
1	1A	305	U	N1-C2-O2	-7.29	117.70	122.80
1	1A	1622	G	N9-C4-C5	7.29	108.31	105.40
1	1A	1975	G	C4-C5-N7	7.29	113.72	110.80
1	2A	1328	G	N9-C4-C5	-7.29	102.48	105.40
1	2A	62	C	C5-C6-N1	-7.29	117.36	121.00
1	2A	676	A	N1-C2-N3	-7.29	125.66	129.30
1	1A	1367	A	C5-C6-N1	7.28	121.34	117.70
1	1A	1671	U	C5-C4-O4	7.28	130.27	125.90
1	1A	2432	A	O5'-P-OP2	7.28	119.44	110.70
1	1A	2823	A	C6-N1-C2	-7.28	114.23	118.60
1	2A	2563	U	C5-C4-O4	7.28	130.27	125.90
1	1A	2440	C	C2-N1-C1'	-7.28	110.79	118.80
1	1A	311	A	OP1-P-OP2	-7.28	108.68	119.60
1	1A	1170	G	N7-C8-N9	7.28	116.74	113.10
1	1A	2120	G	C8-N9-C4	-7.28	103.49	106.40
1	2A	1557	C	O5'-P-OP2	-7.28	99.15	105.70
1	2A	2672	G	O5'-P-OP1	-7.28	99.15	105.70
1	1A	2385	C	OP1-P-OP2	7.28	130.52	119.60
32	2a	730	G	N1-C6-O6	-7.28	115.53	119.90
1	1A	1888	G	C4-C5-N7	7.28	113.71	110.80
1	2A	1584	C	N3-C4-C5	-7.28	118.99	121.90
1	1A	59	U	OP2-P-O3'	7.28	121.20	105.20
1	1A	376	C	C5-C6-N1	-7.28	117.36	121.00
1	1A	1694	C	C6-N1-C2	7.28	123.21	120.30
1	1A	2265	U	C5-C6-N1	-7.28	119.06	122.70
32	1a	719	C	N3-C4-C5	-7.28	118.99	121.90
1	1A	1516	C	O5'-P-OP1	-7.27	99.15	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	783	A	N1-C6-N6	-7.27	114.24	118.60
1	2A	1178	C	C6-N1-C2	-7.27	117.39	120.30
32	2a	802	A	C8-N9-C4	-7.27	102.89	105.80
2	1B	98	G	N9-C4-C5	-7.27	102.49	105.40
1	2A	1667	G	O5'-P-OP1	-7.27	99.16	105.70
32	1a	1520	G	OP1-P-OP2	7.27	130.50	119.60
1	2A	1272	A	O5'-P-OP2	-7.27	99.16	105.70
1	1A	2474	C	N1-C2-O2	7.26	123.26	118.90
32	2a	585	G	C5-C6-N1	7.26	115.13	111.50
1	1A	118	A	C8-N9-C4	7.26	108.70	105.80
32	1a	1495	U	C5-C6-N1	7.26	126.33	122.70
1	1A	390	A	C8-N9-C4	7.26	108.70	105.80
1	1A	1573	G	C2-N3-C4	-7.26	108.27	111.90
1	1A	2406	U	O5'-P-OP1	7.26	119.41	110.70
1	2A	1312	U	C6-N1-C2	-7.26	116.64	121.00
1	2A	1678	G	C4-C5-C6	7.26	123.16	118.80
1	2A	1970	A	O5'-P-OP2	-7.26	99.17	105.70
1	1A	1003	G	C8-N9-C4	7.26	109.30	106.40
1	2A	2690	C	C6-N1-C2	7.26	123.20	120.30
1	1A	635	C	C6-N1-C2	-7.25	117.40	120.30
1	2A	2231	C	N1-C2-O2	-7.25	114.55	118.90
1	1A	1300	U	C6-N1-C2	-7.25	116.65	121.00
1	1A	2433	A	C5-C6-N1	-7.25	114.07	117.70
1	2A	102	G	N3-C4-N9	-7.25	121.65	126.00
1	1A	1609	A	N7-C8-N9	-7.25	110.17	113.80
1	1A	1618	A	C8-N9-C4	7.25	108.70	105.80
1	1A	2065	C	N3-C4-C5	7.25	124.80	121.90
1	2A	684	G	C8-N9-C4	-7.25	103.50	106.40
1	2A	932	G	C6-C5-N7	7.25	134.75	130.40
1	2A	1005	C	N3-C2-O2	-7.25	116.83	121.90
1	1A	972	G	O5'-P-OP1	7.24	119.39	110.70
1	1A	2139	C	N1-C2-O2	7.24	123.25	118.90
1	1A	2484	G	N1-C6-O6	7.24	124.25	119.90
1	2A	1689	A	N1-C6-N6	7.24	122.95	118.60
1	1A	127	A	C4-C5-N7	7.24	114.32	110.70
1	1A	693	C	C6-N1-C2	7.24	123.20	120.30
32	1a	643	C	C6-N1-C2	7.24	123.20	120.30
1	2A	563	G	C2-N3-C4	-7.24	108.28	111.90
1	2A	827	U	C5-C4-O4	-7.24	121.56	125.90
1	1A	2263	C	OP1-P-O3'	7.24	121.12	105.20
1	1A	2455	G	OP1-P-OP2	-7.24	108.75	119.60
1	1A	2646	C	C5-C4-N4	-7.24	115.13	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	463	G	C4-C5-N7	-7.24	107.91	110.80
1	1A	942	G	N7-C8-N9	-7.23	109.48	113.10
1	1A	1410	G	N1-C6-O6	7.23	124.24	119.90
16	1U	18	LEU	CA-CB-CG	-7.23	98.66	115.30
1	1A	466	A	OP2-P-O3'	7.23	121.11	105.20
1	1A	1660	C	N1-C2-O2	7.23	123.24	118.90
1	2A	351	G	N3-C4-C5	-7.23	124.98	128.60
1	2A	1031	G	N7-C8-N9	-7.23	109.48	113.10
1	1A	1519	G	C8-N9-C4	-7.23	103.51	106.40
1	1A	119	A	N1-C6-N6	-7.23	114.26	118.60
1	2A	1255	U	O5'-P-OP1	-7.22	99.20	105.70
1	1A	945	A	O5'-P-OP1	-7.22	99.20	105.70
1	1A	2445	G	N9-C4-C5	7.22	108.29	105.40
1	2A	932	G	C5-C6-O6	7.22	132.93	128.60
1	1A	960	A	C4-C5-N7	7.22	114.31	110.70
1	1A	1964	G	N3-C4-N9	7.22	130.33	126.00
1	2A	2562	U	N3-C4-C5	-7.22	110.27	114.60
1	2A	2701	C	N3-C2-O2	-7.22	116.84	121.90
1	2A	1937	A	C8-N9-C4	7.22	108.69	105.80
1	1A	2258	C	C2-N1-C1'	7.22	126.74	118.80
1	2A	1626	G	N3-C4-N9	-7.22	121.67	126.00
1	2A	2319	G	C8-N9-C1'	-7.22	117.62	127.00
1	1A	2252	G	C4-C5-N7	7.21	113.69	110.80
1	1A	2820	A	C8-N9-C4	7.21	108.69	105.80
1	1A	2859	G	C8-N9-C4	7.21	109.29	106.40
32	2a	1391	U	C5-C6-N1	-7.21	119.09	122.70
1	1A	2172	U	C5-C4-O4	7.21	130.23	125.90
32	1a	1319	A	C8-N9-C4	-7.21	102.92	105.80
1	1A	1625	C	N3-C4-N4	-7.21	112.95	118.00
1	1A	2231	C	C4-C5-C6	7.21	121.00	117.40
1	2A	784	A	N1-C6-N6	-7.21	114.27	118.60
1	2A	2435	A	N1-C2-N3	7.21	132.90	129.30
1	1A	329	G	N7-C8-N9	-7.21	109.50	113.10
1	1A	1164	G	O5'-P-OP2	-7.21	99.22	105.70
1	1A	2633	G	C5-C6-O6	7.21	132.92	128.60
1	2A	1471	A	C4-C5-C6	7.21	120.60	117.00
32	2a	343	U	N3-C4-O4	-7.21	114.36	119.40
32	2a	442	C	C5-C6-N1	7.21	124.60	121.00
1	1A	1607	C	C5-C4-N4	-7.20	115.16	120.20
1	2A	620	G	N9-C4-C5	7.20	108.28	105.40
1	2A	2086	U	O5'-P-OP2	-7.20	99.22	105.70
1	2A	2494	G	C8-N9-C4	7.20	109.28	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	454	C	N1-C2-O2	7.20	123.22	118.90
1	1A	391	G	N1-C2-N3	7.20	128.22	123.90
1	1A	43	A	C2-N3-C4	-7.20	107.00	110.60
1	1A	285	C	C5-C6-N1	-7.20	117.40	121.00
1	1A	335	C	C5-C6-N1	7.20	124.60	121.00
32	1a	618	C	C6-N1-C2	-7.20	117.42	120.30
1	2A	1626	G	C5-C6-N1	-7.20	107.90	111.50
1	2A	90	U	N3-C2-O2	-7.20	117.16	122.20
32	2a	585	G	N1-C6-O6	-7.20	115.58	119.90
32	1a	1276	G	C8-N9-C4	-7.20	103.52	106.40
1	1A	1234	U	C5-C4-O4	7.19	130.22	125.90
1	1A	1672	C	O5'-P-OP1	-7.19	99.23	105.70
2	2B	98	G	C4-C5-N7	-7.19	107.92	110.80
1	1A	1672	C	C4-C5-C6	7.19	121.00	117.40
1	1A	2456	C	C6-N1-C2	7.19	123.18	120.30
1	1A	2539	C	C5-C6-N1	-7.19	117.40	121.00
1	2A	228	A	C4-C5-N7	7.19	114.30	110.70
1	2A	1668	A	O5'-P-OP2	-7.19	99.23	105.70
1	2A	1926	U	C5-C4-O4	7.19	130.22	125.90
1	1A	45	C	C2-N1-C1'	-7.19	110.89	118.80
1	1A	838	C	OP2-P-O3'	7.19	121.02	105.20
32	2a	898	G	N3-C4-C5	7.19	132.19	128.60
1	1A	1516	C	N3-C4-C5	-7.19	119.03	121.90
1	1A	1340	U	N3-C4-O4	7.19	124.43	119.40
1	1A	2522	U	C5-C6-N1	-7.19	119.11	122.70
32	1a	1367	C	C6-N1-C2	-7.18	117.43	120.30
1	2A	2038	G	C8-N9-C4	7.18	109.27	106.40
1	2A	351	G	N3-C4-N9	7.18	130.31	126.00
1	1A	1607	C	N3-C4-N4	7.18	123.03	118.00
1	2A	1049	C	N3-C4-C5	-7.18	119.03	121.90
1	1A	1320	C	N1-C2-O2	-7.18	114.59	118.90
1	1A	1792	G	N3-C4-N9	-7.17	121.70	126.00
1	1A	2015	A	C2-N3-C4	-7.17	107.01	110.60
1	1A	2162	G	N3-C4-C5	-7.17	125.01	128.60
1	1A	2547	U	N1-C2-N3	7.17	119.20	114.90
1	2A	2111	C	C5-C6-N1	7.17	124.59	121.00
1	2A	1926	U	N1-C2-N3	7.17	119.20	114.90
1	1A	1338	G	C5-C6-O6	-7.17	124.30	128.60
2	1B	77	U	OP1-P-O3'	-7.17	89.43	105.20
1	2A	1997	G	O5'-P-OP1	-7.17	99.25	105.70
32	2a	880	C	C6-N1-C2	7.17	123.17	120.30
1	2A	271	A	N1-C6-N6	7.17	122.90	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	566	U	C5-C6-N1	-7.17	119.12	122.70
1	1A	2045	C	C6-N1-C2	7.17	123.17	120.30
1	1A	2422	A	C5-C6-N6	7.17	129.43	123.70
1	1A	2764	A	N1-C6-N6	-7.16	114.30	118.60
1	1A	1653	G	N3-C4-C5	-7.16	125.02	128.60
1	1A	2501	C	N1-C2-O2	-7.16	114.60	118.90
1	2A	2142	C	C5-C6-N1	7.16	124.58	121.00
1	1A	706	A	C8-N9-C4	7.16	108.66	105.80
1	1A	733	G	N3-C2-N2	7.16	124.91	119.90
1	2A	2372	G	C6-C5-N7	-7.16	126.11	130.40
23	11	41	ARG	NE-CZ-NH2	-7.16	116.72	120.30
32	1a	346	G	C6-N1-C2	-7.16	120.81	125.10
32	1a	533	A	N9-C4-C5	-7.15	102.94	105.80
32	2a	121	C	C6-N1-C2	7.15	123.16	120.30
1	1A	57	C	N3-C2-O2	7.15	126.91	121.90
1	1A	739	G	OP2-P-O3'	-7.15	89.47	105.20
1	1A	2088	G	O5'-P-OP2	7.15	119.28	110.70
1	1A	2741	A	N1-C6-N6	7.15	122.89	118.60
32	2a	886	G	N1-C6-O6	7.15	124.19	119.90
1	2A	1663	C	C5-C6-N1	-7.15	117.43	121.00
1	1A	530	G	C5-C6-N1	7.15	115.07	111.50
1	2A	301	G	C8-N9-C4	7.15	109.26	106.40
32	1a	521	G	N3-C4-C5	-7.15	125.03	128.60
1	1A	2499	C	OP1-P-OP2	-7.14	108.88	119.60
1	1A	2553	G	C2-N3-C4	7.14	115.47	111.90
1	2A	2789	C	C6-N1-C1'	7.14	129.37	120.80
4	1E	149	ARG	NE-CZ-NH2	-7.14	116.73	120.30
32	1a	795	C	N1-C2-O2	-7.14	114.61	118.90
32	2a	115	G	P-O3'-C3'	7.14	128.27	119.70
1	1A	272	G	N3-C4-C5	-7.14	125.03	128.60
1	2A	461	C	N1-C2-O2	-7.14	114.62	118.90
1	2A	1783	A	N9-C4-C5	7.14	108.66	105.80
1	1A	904	C	N3-C4-C5	7.14	124.75	121.90
1	1A	2451	A	C8-N9-C4	-7.14	102.95	105.80
1	1A	2718	G	N3-C2-N2	-7.14	114.91	119.90
11	2P	90	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	1A	777	A	N1-C6-N6	-7.13	114.32	118.60
32	1a	1331	G	O4'-C1'-N9	7.13	113.91	108.20
1	2A	391	G	C4-N9-C1'	7.13	135.77	126.50
1	1A	1839	G	N3-C4-N9	7.13	130.28	126.00
2	1B	118	G	C8-N9-C4	7.13	109.25	106.40
1	1A	513	A	C5-C6-N6	-7.13	118.00	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2D	242	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	1A	867	C	N1-C2-O2	-7.13	114.62	118.90
1	1A	191	A	OP1-P-O3'	-7.13	89.52	105.20
1	1A	1331	A	OP2-P-O3'	7.13	120.88	105.20
1	2A	856	C	N3-C4-C5	-7.13	119.05	121.90
1	2A	2476	A	N1-C2-N3	7.13	132.86	129.30
32	2a	509	A	C8-N9-C4	-7.13	102.95	105.80
32	2a	913	A	P-O3'-C3'	7.13	128.25	119.70
1	2A	463	G	C5-C6-N1	-7.13	107.94	111.50
1	2A	1372	U	C6-N1-C2	-7.13	116.72	121.00
1	1A	1824	G	N9-C4-C5	-7.12	102.55	105.40
1	2A	1518	U	O5'-P-OP2	-7.12	99.29	105.70
1	1A	570	G	N3-C2-N2	7.12	124.89	119.90
1	1A	2025	C	OP2-P-O3'	7.12	120.87	105.20
1	2A	1830	C	C6-N1-C2	7.12	123.15	120.30
1	1A	411	G	N3-C4-C5	-7.12	125.04	128.60
1	1A	986	C	C5-C6-N1	7.12	124.56	121.00
1	1A	1198	U	N3-C2-O2	-7.12	117.22	122.20
1	1A	1520	G	N1-C6-O6	-7.12	115.63	119.90
32	2a	764	C	N1-C2-O2	7.12	123.17	118.90
32	2a	1499	A	N9-C4-C5	-7.12	102.95	105.80
1	1A	1210	A	N1-C2-N3	7.12	132.86	129.30
1	1A	1406	U	N1-C2-N3	7.12	119.17	114.90
1	2A	2579	C	C4-C5-C6	-7.12	113.84	117.40
1	1A	513	A	C5-C6-N1	7.12	121.26	117.70
1	1A	2429	G	N3-C4-C5	-7.12	125.04	128.60
1	2A	1823	G	O5'-P-OP2	7.12	119.24	110.70
1	1A	678	C	C4-C5-C6	7.11	120.96	117.40
1	2A	1400	G	C8-N9-C4	-7.11	103.56	106.40
32	2a	525	C	C2-N3-C4	7.11	123.46	119.90
1	1A	1137	G	C6-C5-N7	-7.11	126.13	130.40
32	1a	869	G	O5'-P-OP2	7.11	119.23	110.70
1	1A	1203	G	N9-C4-C5	-7.11	102.56	105.40
32	1a	503	C	C6-N1-C2	-7.11	117.46	120.30
32	2a	1300	G	N1-C6-O6	7.11	124.16	119.90
1	1A	253	C	C6-N1-C2	7.11	123.14	120.30
1	1A	892	G	C8-N9-C4	7.11	109.24	106.40
1	1A	960	A	N9-C4-C5	-7.11	102.96	105.80
1	1A	1320	C	C5-C6-N1	-7.11	117.45	121.00
1	1A	1674	G	O4'-C1'-N9	-7.11	102.52	108.20
32	1a	700	G	O5'-P-OP2	-7.11	99.31	105.70
1	1A	446	G	C2-N3-C4	-7.10	108.35	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	898	G	N1-C6-O6	7.10	124.16	119.90
32	2a	1060	C	C6-N1-C2	-7.10	117.46	120.30
1	1A	185	U	N1-C2-N3	7.10	119.16	114.90
1	1A	2246	G	N7-C8-N9	-7.10	109.55	113.10
1	1A	2417	C	O5'-P-OP2	-7.10	99.31	105.70
1	1A	127	A	C5-C6-N1	7.10	121.25	117.70
32	2a	398	C	C5-C4-N4	7.10	125.17	120.20
1	2A	1416	G	C4-N9-C1'	-7.10	117.28	126.50
1	1A	390	A	N1-C6-N6	7.09	122.86	118.60
1	1A	391	G	N1-C6-O6	7.09	124.16	119.90
1	2A	2755	C	C2-N3-C4	7.09	123.45	119.90
1	1A	329	G	O4'-C1'-N9	-7.09	102.53	108.20
32	1a	1505	G	C8-N9-C1'	7.09	136.22	127.00
1	2A	1040	C	N1-C2-O2	7.09	123.16	118.90
32	1a	224	C	N3-C4-C5	-7.09	119.06	121.90
1	2A	2032	G	C5-N7-C8	7.09	107.84	104.30
32	1a	1319	A	N9-C4-C5	7.09	108.64	105.80
1	1A	242	G	C8-N9-C4	7.09	109.23	106.40
2	2B	27	C	C6-N1-C2	-7.09	117.47	120.30
1	1A	1780	A	O5'-P-OP1	-7.08	99.33	105.70
1	1A	1161	C	N3-C4-C5	7.08	124.73	121.90
1	1A	1319	G	C8-N9-C4	-7.08	103.57	106.40
1	2A	1965	C	C5-C4-N4	-7.08	115.24	120.20
1	2A	2476	A	C8-N9-C4	-7.08	102.97	105.80
1	1A	45	C	N1-C2-N3	-7.08	114.24	119.20
1	1A	1008	C	N1-C2-O2	7.08	123.15	118.90
1	1A	1203	G	C6-C5-N7	-7.08	126.15	130.40
1	1A	1593	G	C5-C6-N1	-7.08	107.96	111.50
2	1B	106	G	N7-C8-N9	-7.08	109.56	113.10
32	1a	427	U	C6-N1-C2	-7.08	116.75	121.00
32	1a	1107	C	C6-N1-C2	-7.08	117.47	120.30
1	1A	228	A	C6-C5-N7	-7.07	127.35	132.30
1	2A	812	C	N3-C4-C5	-7.07	119.07	121.90
1	2A	2496	C	N3-C2-O2	-7.07	116.95	121.90
1	2A	959	A	N3-C4-C5	-7.07	121.85	126.80
1	1A	467	G	O5'-P-OP1	7.07	119.18	110.70
1	2A	630	G	C8-N9-C4	7.07	109.23	106.40
1	2A	1363	C	N3-C2-O2	-7.07	116.95	121.90
1	1A	536	A	C5-N7-C8	-7.07	100.37	103.90
1	1A	570	G	C5-C6-O6	7.07	132.84	128.60
1	1A	2498	C	P-O3'-C3'	-7.07	111.22	119.70
1	1A	2614	A	C8-N9-C4	7.07	108.63	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	959	A	C4-C5-C6	7.07	120.53	117.00
1	2A	2562	U	O5'-P-OP2	-7.07	99.34	105.70
1	1A	386	G	N1-C6-O6	7.07	124.14	119.90
2	1B	118	G	C4-N9-C1'	-7.07	117.31	126.50
1	1A	1274	A	N9-C4-C5	-7.06	102.97	105.80
1	1A	2070	G	N1-C2-N2	-7.06	109.84	116.20
1	2A	967	C	N1-C2-O2	-7.06	114.66	118.90
1	1A	25	U	C5-C4-O4	-7.06	121.66	125.90
1	1A	885	C	C6-N1-C2	-7.06	117.48	120.30
1	1A	1993	U	OP2-P-O3'	7.06	120.73	105.20
1	1A	2071	A	C8-N9-C4	7.06	108.62	105.80
1	2A	2538	C	N3-C4-C5	7.06	124.72	121.90
1	1A	27	G	O4'-C1'-N9	7.06	113.85	108.20
1	1A	1268	A	C2-N3-C4	-7.06	107.07	110.60
1	1A	2003	G	N1-C2-N3	7.06	128.13	123.90
1	1A	2250	G	N9-C4-C5	7.06	108.22	105.40
1	1A	2512	C	N1-C2-O2	-7.06	114.67	118.90
32	1a	481	G	N1-C6-O6	7.06	124.13	119.90
1	2A	2828	C	C6-N1-C2	7.06	123.12	120.30
32	2a	244	U	C6-N1-C2	7.06	125.23	121.00
1	1A	1632	A	C5-C6-N1	-7.05	114.17	117.70
32	1a	623	C	C6-N1-C2	-7.05	117.48	120.30
1	1A	1135	C	N1-C2-O2	7.05	123.13	118.90
1	2A	666	G	C4-C5-N7	7.05	113.62	110.80
1	1A	2052	G	C6-C5-N7	-7.05	126.17	130.40
1	2A	810	U	C5-C4-O4	-7.05	121.67	125.90
1	2A	97	C	C5-C6-N1	-7.05	117.47	121.00
1	1A	2246	G	C5-C6-N1	7.05	115.02	111.50
32	1a	911	U	C5-C4-O4	7.05	130.13	125.90
1	2A	1937	A	N7-C8-N9	-7.05	110.28	113.80
1	1A	706	A	C2-N3-C4	-7.05	107.08	110.60
1	1A	1800	C	C6-N1-C1'	7.05	129.26	120.80
1	2A	1190	G	N3-C4-N9	7.05	130.23	126.00
1	2A	2577	A	C8-N9-C4	-7.05	102.98	105.80
32	2a	815	A	C8-N9-C4	7.05	108.62	105.80
1	1A	983	A	OP2-P-O3'	7.04	120.70	105.20
1	1A	2512	C	N3-C4-C5	-7.04	119.08	121.90
32	1a	1408	A	C8-N9-C4	7.04	108.62	105.80
1	1A	508	G	O5'-P-OP1	-7.04	99.36	105.70
1	1A	775	G	C8-N9-C4	7.04	109.22	106.40
1	2A	1029	A	N1-C6-N6	7.04	122.83	118.60
2	2B	114	C	C6-N1-C2	-7.04	117.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	191	A	OP2-P-O3'	7.04	120.69	105.20
1	1A	250	G	N3-C4-N9	-7.04	121.78	126.00
1	1A	2000	G	N1-C6-O6	7.04	124.12	119.90
1	2A	2439	A	O5'-P-OP2	-7.04	99.36	105.70
2	2B	71	C	O5'-P-OP1	-7.04	99.36	105.70
32	1a	804	U	O5'-P-OP1	7.04	119.15	110.70
1	2A	2518	A	OP1-P-OP2	-7.04	109.04	119.60
1	1A	767	U	C6-N1-C2	-7.04	116.78	121.00
1	1A	1248	G	N1-C6-O6	7.04	124.12	119.90
1	1A	2252	G	C5-C6-O6	-7.04	124.38	128.60
2	1B	105	A	N9-C4-C5	-7.04	102.99	105.80
1	2A	392	C	O5'-P-OP1	-7.04	99.37	105.70
1	1A	2507	C	N1-C2-O2	-7.03	114.68	118.90
32	1a	1287	A	C5-C6-N1	-7.03	114.18	117.70
1	1A	2384	G	O5'-P-OP2	-7.03	99.37	105.70
1	1A	2746	U	C5-C4-O4	7.03	130.12	125.90
1	2A	2012	G	N1-C2-N3	7.03	128.12	123.90
32	2a	710	G	N1-C6-O6	7.03	124.12	119.90
1	1A	347	A	C2-N3-C4	-7.03	107.08	110.60
1	1A	996	A	C2-N3-C4	7.03	114.11	110.60
1	1A	2275	C	N3-C4-C5	-7.03	119.09	121.90
1	1A	2647	U	C5-C6-N1	-7.03	119.19	122.70
1	1A	1607	C	OP1-P-O3'	7.03	120.66	105.20
2	1B	118	G	N3-C4-N9	-7.03	121.78	126.00
1	2A	58	G	C8-N9-C4	-7.03	103.59	106.40
32	1a	811	C	OP2-P-O3'	7.03	120.66	105.20
32	2a	346	G	N1-C2-N2	-7.03	109.88	116.20
32	2a	1228	C	C6-N1-C2	-7.03	117.49	120.30
32	2a	1456	G	C8-N9-C4	7.03	109.21	106.40
1	1A	21	A	N1-C6-N6	7.03	122.82	118.60
1	1A	1651	G	N9-C4-C5	-7.02	102.59	105.40
1	2A	1690	A	C8-N9-C4	7.02	108.61	105.80
1	1A	673	C	C6-N1-C1'	-7.02	112.37	120.80
1	1A	1384	A	C8-N9-C4	-7.02	102.99	105.80
1	1A	1581	G	N7-C8-N9	7.02	116.61	113.10
32	1a	299	G	C4-C5-N7	7.02	113.61	110.80
1	1A	681	G	C5-C6-N1	-7.02	107.99	111.50
32	2a	338	A	C8-N9-C4	-7.02	102.99	105.80
1	1A	1274	A	C2-N3-C4	-7.02	107.09	110.60
1	2A	1264	G	C6-C5-N7	-7.02	126.19	130.40
1	2A	1934	C	C5-C6-N1	-7.02	117.49	121.00
1	1A	1452	A	C5-C6-N6	-7.02	118.09	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2028	U	C2-N1-C1'	-7.02	109.28	117.70
1	1A	442	G	C8-N9-C4	-7.02	103.59	106.40
1	1A	2575	C	OP1-P-O3'	7.02	120.64	105.20
1	2A	252	G	N1-C6-O6	-7.02	115.69	119.90
1	1A	2679	A	C8-N9-C4	7.01	108.61	105.80
1	1A	1002	G	C5-C6-N1	-7.01	107.99	111.50
1	1A	130	C	N3-C4-C5	7.01	124.70	121.90
1	1A	2419	U	OP1-P-O3'	7.01	120.62	105.20
1	2A	1663	C	N3-C4-C5	7.01	124.70	121.90
1	1A	789	A	N1-C2-N3	7.01	132.81	129.30
1	1A	911	A	C6-C5-N7	-7.01	127.39	132.30
1	2A	116	C	N1-C2-O2	-7.01	114.69	118.90
1	1A	941	A	N7-C8-N9	7.01	117.30	113.80
32	1a	911	U	N3-C2-O2	-7.01	117.30	122.20
1	2A	127	A	N9-C4-C5	-7.01	103.00	105.80
1	2A	2242	G	N1-C6-O6	7.01	124.10	119.90
2	2B	27	C	N3-C2-O2	-7.01	117.00	121.90
32	2a	993	G	N3-C4-N9	7.01	130.20	126.00
1	1A	1266	G	C8-N9-C4	7.00	109.20	106.40
32	1a	186	C	C6-N1-C2	-7.00	117.50	120.30
1	2A	2735	G	C5-C6-N1	7.00	115.00	111.50
1	1A	920	G	C2-N3-C4	-7.00	108.40	111.90
1	1A	1695	G	C5-C6-N1	-7.00	108.00	111.50
32	1a	1488	G	C8-N9-C4	7.00	109.20	106.40
1	2A	819	A	C8-N9-C4	-7.00	103.00	105.80
2	1B	63	G	C8-N9-C4	7.00	109.20	106.40
1	1A	800	A	OP1-P-OP2	7.00	130.10	119.60
1	1A	2418	A	C8-N9-C4	7.00	108.60	105.80
1	2A	1667	G	C5-C6-O6	-7.00	124.40	128.60
32	2a	244	U	N3-C4-C5	7.00	118.80	114.60
1	1A	128	C	C2-N3-C4	-7.00	116.40	119.90
32	1a	1479	C	N1-C2-O2	-7.00	114.70	118.90
1	2A	446	G	C8-N9-C4	7.00	109.20	106.40
1	2A	1606	G	N3-C4-N9	7.00	130.20	126.00
32	2a	246	A	O5'-P-OP2	-7.00	99.40	105.70
1	2A	2575	C	C4-C5-C6	7.00	120.90	117.40
1	1A	252	G	N9-C4-C5	6.99	108.20	105.40
1	2A	456	C	C6-N1-C2	6.99	123.10	120.30
1	1A	1792	G	C4-C5-N7	-6.99	108.00	110.80
1	1A	2440	C	N3-C4-C5	-6.99	119.10	121.90
1	1A	1131	G	C6-N1-C2	6.99	129.29	125.10
1	1A	2088	G	C5-C6-O6	-6.99	124.41	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	750	A	N1-C2-N3	6.99	132.79	129.30
1	1A	1213	A	N1-C2-N3	6.99	132.79	129.30
1	1A	1661	G	C8-N9-C4	6.99	109.20	106.40
1	1A	2573	C	C5-C4-N4	-6.99	115.31	120.20
32	2a	999	C	N1-C2-O2	6.99	123.09	118.90
1	1A	2509	G	O5'-P-OP1	-6.99	99.41	105.70
32	1a	442	C	C6-N1-C2	-6.99	117.50	120.30
18	2W	23	LEU	CA-CB-CG	6.99	131.37	115.30
1	2A	1184	G	N3-C4-C5	6.99	132.09	128.60
1	2A	2065	C	N3-C4-C5	6.99	124.69	121.90
32	2a	972	C	C5-C6-N1	6.99	124.49	121.00
1	1A	255	A	N1-C2-N3	6.98	132.79	129.30
1	1A	1052	C	C5-C6-N1	6.98	124.49	121.00
1	1A	1695	G	N9-C4-C5	-6.98	102.61	105.40
1	1A	2766	G	N3-C2-N2	-6.98	115.01	119.90
32	1a	73	G	C6-C5-N7	6.98	134.59	130.40
32	1a	823	G	N7-C8-N9	-6.98	109.61	113.10
1	2A	272	G	C5-C6-O6	-6.98	124.41	128.60
1	2A	1684	C	N3-C4-C5	-6.98	119.11	121.90
1	1A	202	U	OP1-P-OP2	6.98	130.07	119.60
1	1A	2003	G	C6-C5-N7	-6.98	126.21	130.40
1	1A	2062	A	N1-C6-N6	6.98	122.79	118.60
32	1a	292	G	O5'-P-OP2	-6.98	99.42	105.70
32	1a	380	G	N1-C6-O6	-6.98	115.71	119.90
1	2A	1653	G	C8-N9-C4	6.98	109.19	106.40
1	1A	207	A	C5-C6-N6	-6.98	118.12	123.70
1	1A	298	G	C4-C5-N7	-6.98	108.01	110.80
1	2A	2507	C	C6-N1-C2	-6.98	117.51	120.30
32	1a	784	C	N1-C2-O2	6.98	123.09	118.90
1	2A	912	C	C5-C6-N1	6.98	124.49	121.00
1	2A	2018	G	O5'-P-OP2	-6.97	99.42	105.70
1	1A	408	G	N3-C4-N9	6.97	130.18	126.00
1	1A	574	C	O5'-P-OP1	-6.97	99.43	105.70
1	1A	2568	C	N3-C2-O2	6.97	126.78	121.90
1	1A	2779	U	N1-C2-O2	6.97	127.68	122.80
2	1B	13	A	N7-C8-N9	-6.97	110.31	113.80
1	2A	15	G	N9-C4-C5	-6.97	102.61	105.40
1	1A	777	A	OP1-P-OP2	6.97	130.06	119.60
1	1A	2781	A	O5'-P-OP2	-6.97	99.43	105.70
1	1A	2082	A	O5'-P-OP1	6.97	119.06	110.70
2	1B	60	C	C6-N1-C2	-6.97	117.51	120.30
1	2A	2572	A	C5-C6-N6	6.97	129.27	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1164	G	C5-C6-O6	6.97	132.78	128.60
1	1A	1601	G	N1-C6-O6	6.97	124.08	119.90
1	1A	2445	G	N3-C4-C5	-6.97	125.12	128.60
1	1A	2701	C	C2-N3-C4	-6.96	116.42	119.90
32	2a	577	G	N9-C4-C5	-6.96	102.61	105.40
1	1A	530	G	N1-C6-O6	-6.96	115.72	119.90
1	2A	141	A	N9-C4-C5	-6.96	103.02	105.80
1	1A	997	G	N7-C8-N9	-6.96	109.62	113.10
1	2A	69	C	C6-N1-C2	6.96	123.08	120.30
1	1A	1195	G	N3-C2-N2	-6.96	115.03	119.90
1	1A	2008	C	N3-C4-C5	-6.96	119.12	121.90
1	2A	948	G	N3-C4-N9	-6.96	121.83	126.00
1	2A	1325	G	N3-C2-N2	6.96	124.77	119.90
1	2A	2514	U	C6-N1-C2	6.96	125.17	121.00
32	2a	544	G	C8-N9-C4	6.96	109.18	106.40
1	1A	1413	G	O5'-P-OP2	6.96	119.05	110.70
32	1a	890	G	O4'-C1'-N9	6.96	113.76	108.20
1	2A	2078	C	N1-C2-O2	-6.96	114.73	118.90
1	1A	214	G	O5'-P-OP2	-6.95	99.44	105.70
1	2A	1266	G	C8-N9-C4	6.95	109.18	106.40
1	2A	2237	G	N3-C4-N9	-6.95	121.83	126.00
1	1A	2004	G	OP1-P-OP2	6.95	130.03	119.60
1	1A	2081	C	C5-C6-N1	-6.95	117.53	121.00
1	2A	102	G	N3-C4-C5	6.95	132.07	128.60
32	2a	841	U	C5-C6-N1	6.95	126.17	122.70
1	1A	840	C	N1-C2-O2	-6.95	114.73	118.90
1	1A	1187	G	C2-N3-C4	6.95	115.37	111.90
32	2a	829	G	C8-N9-C4	-6.95	103.62	106.40
1	1A	1573	G	N3-C4-N9	-6.95	121.83	126.00
1	2A	1897	G	C2-N3-C4	-6.94	108.43	111.90
1	1A	2512	C	N3-C2-O2	6.94	126.76	121.90
32	1a	1442(B)	A	N1-C6-N6	6.94	122.77	118.60
1	2A	467	G	N7-C8-N9	-6.94	109.63	113.10
1	1A	130	C	C2-N3-C4	-6.94	116.43	119.90
1	1A	1153	C	C5-C6-N1	6.94	124.47	121.00
32	1a	1102	A	C8-N9-C4	-6.94	103.02	105.80
1	2A	768	G	N1-C6-O6	6.94	124.06	119.90
1	2A	1249	U	O5'-P-OP1	-6.94	99.45	105.70
1	1A	1308	A	C4-C5-C6	6.94	120.47	117.00
1	1A	2040	C	N3-C4-N4	6.94	122.86	118.00
1	2A	669	G	N1-C2-N2	6.94	122.44	116.20
1	1A	559	G	N1-C6-O6	6.94	124.06	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	752	A	C5-C6-N6	-6.94	118.15	123.70
1	2A	1176	G	C8-N9-C4	6.94	109.17	106.40
1	1A	1347	G	C8-N9-C4	-6.94	103.63	106.40
1	1A	2483	C	C6-N1-C1'	-6.94	112.48	120.80
1	1A	945	A	N7-C8-N9	-6.93	110.33	113.80
1	1A	1008	C	C5-C6-N1	6.93	124.47	121.00
1	1A	663	G	N9-C4-C5	6.93	108.17	105.40
1	1A	685	A	N9-C4-C5	6.93	108.57	105.80
1	1A	1395	A	N7-C8-N9	-6.93	110.33	113.80
1	2A	980	A	C5-N7-C8	-6.93	100.43	103.90
2	1B	1	U	C5-C6-N1	6.93	126.16	122.70
1	2A	1260	G	C8-N9-C4	6.93	109.17	106.40
32	2a	1261	A	N1-C6-N6	6.93	122.76	118.60
1	1A	21	A	C5-C6-N6	-6.93	118.16	123.70
1	1A	976	C	C4-C5-C6	-6.93	113.94	117.40
32	1a	522	C	C2-N1-C1'	-6.93	111.18	118.80
1	2A	1363	C	N1-C2-O2	6.93	123.06	118.90
1	1A	645	C	C2-N1-C1'	6.92	126.42	118.80
1	1A	934	G	C8-N9-C1'	-6.92	118.00	127.00
1	1A	2399	G	N1-C6-O6	-6.92	115.75	119.90
1	1A	2657	A	C5-C6-N1	6.92	121.16	117.70
2	1B	53	A	C8-N9-C4	-6.92	103.03	105.80
1	2A	2178	C	C6-N1-C2	-6.92	117.53	120.30
1	1A	12	U	N1-C2-O2	6.92	127.64	122.80
1	1A	1133	U	N1-C2-O2	-6.92	117.96	122.80
1	1A	1466	G	N9-C4-C5	6.92	108.17	105.40
1	2A	1046	A	C8-N9-C4	-6.92	103.03	105.80
1	2A	2391	G	C8-N9-C4	6.92	109.17	106.40
1	2A	2720	U	C5-C4-O4	6.92	130.05	125.90
1	1A	109	G	C6-C5-N7	6.92	134.55	130.40
1	2A	341	G	O5'-P-OP2	-6.92	99.47	105.70
2	2B	115	G	N1-C6-O6	6.92	124.05	119.90
1	1A	1663	C	N3-C4-N4	6.92	122.84	118.00
1	1A	189	G	C5-C6-O6	-6.91	124.45	128.60
1	1A	838	C	N3-C4-C5	-6.91	119.14	121.90
1	2A	801	G	N3-C4-N9	-6.91	121.85	126.00
1	2A	871	U	O5'-P-OP2	6.91	119.00	110.70
1	2A	2099	U	C6-N1-C2	-6.91	116.85	121.00
32	2a	1317	C	C6-N1-C2	6.91	123.07	120.30
1	1A	599	G	N1-C6-O6	6.91	124.05	119.90
1	1A	1163	G	C5-C6-O6	-6.91	124.45	128.60
1	1A	330	A	N1-C6-N6	6.91	122.75	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	498	G	N1-C6-O6	6.91	124.05	119.90
1	1A	694	U	N1-C2-O2	6.91	127.64	122.80
1	1A	2069	G	C4-C5-N7	-6.91	108.04	110.80
32	1a	1434	A	N7-C8-N9	-6.91	110.35	113.80
1	2A	925	C	N3-C4-C5	6.91	124.66	121.90
1	2A	1067	A	C2-N3-C4	6.91	114.05	110.60
1	1A	1210	A	P-O3'-C3'	6.91	127.99	119.70
1	1A	2069	G	N1-C6-O6	-6.91	115.76	119.90
1	1A	2407	G	C8-N9-C1'	-6.91	118.02	127.00
1	1A	2200	C	O5'-P-OP2	-6.91	99.49	105.70
1	1A	2748	A	N1-C6-N6	6.91	122.74	118.60
32	1a	790	A	C5-C6-N1	-6.91	114.25	117.70
32	1a	1287	A	C5-C6-N6	6.91	129.22	123.70
32	1a	1506	U	C5-C4-O4	-6.90	121.76	125.90
1	2A	1626	G	C8-N9-C4	-6.90	103.64	106.40
1	2A	1964	G	O5'-P-OP1	-6.90	99.49	105.70
1	2A	2822	G	N9-C4-C5	-6.90	102.64	105.40
1	1A	2082	A	C8-N9-C4	6.90	108.56	105.80
1	1A	2696	U	O5'-P-OP2	-6.90	99.49	105.70
32	1a	841	U	N3-C2-O2	-6.90	117.37	122.20
32	1a	1445	C	C6-N1-C2	6.90	123.06	120.30
32	2a	30	U	OP1-P-OP2	6.90	129.95	119.60
1	1A	572	A	N1-C2-N3	6.90	132.75	129.30
32	1a	1018	C	C5-C6-N1	6.90	124.45	121.00
1	2A	491	G	C8-N9-C4	-6.90	103.64	106.40
1	1A	312	G	N1-C6-O6	6.89	124.04	119.90
32	1a	401	C	C6-N1-C2	-6.89	117.54	120.30
1	1A	31	C	N1-C2-O2	-6.89	114.77	118.90
1	1A	224	G	O5'-P-OP2	-6.89	99.50	105.70
1	1A	1562	A	O5'-P-OP1	-6.89	99.50	105.70
1	1A	1626	G	O5'-P-OP2	6.89	118.97	110.70
1	1A	2705	A	O5'-P-OP2	6.89	118.97	110.70
1	1A	2789	C	C5-C6-N1	-6.89	117.55	121.00
1	2A	139(A)	G	C5-N7-C8	6.89	107.75	104.30
1	1A	734	A	N1-C6-N6	6.89	122.73	118.60
1	2A	2738	A	N1-C6-N6	-6.89	114.47	118.60
1	1A	1434	A	C5-C6-N6	6.89	129.21	123.70
1	2A	608	A	C8-N9-C4	-6.89	103.05	105.80
32	2a	768	A	C2-N3-C4	-6.89	107.16	110.60
1	1A	1668	A	C8-N9-C4	-6.89	103.05	105.80
1	1A	2714	G	C8-N9-C4	-6.89	103.64	106.40
32	1a	1259	C	C6-N1-C2	-6.89	117.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1853	A	OP1-P-OP2	6.89	129.93	119.60
32	2a	1465	C	C2-N3-C4	-6.89	116.46	119.90
1	2A	257	A	C6-N1-C2	-6.88	114.47	118.60
1	2A	1297	C	OP1-P-O3'	6.88	120.35	105.20
1	1A	670	A	N1-C6-N6	6.88	122.73	118.60
1	2A	866	A	N1-C6-N6	6.88	122.73	118.60
1	2A	207	A	C2-N3-C4	-6.88	107.16	110.60
2	2B	115	G	C5-C6-O6	-6.88	124.47	128.60
1	1A	1283	G	C5-N7-C8	6.88	107.74	104.30
1	1A	1660	C	N3-C4-N4	-6.88	113.18	118.00
1	1A	1025	G	C5-C6-O6	6.88	132.73	128.60
1	1A	1003	G	N7-C8-N9	-6.88	109.66	113.10
2	1B	51	G	N1-C6-O6	6.88	124.03	119.90
32	1a	26	A	N1-C2-N3	6.88	132.74	129.30
1	1A	1598	C	N1-C2-O2	-6.88	114.78	118.90
1	1A	1955	U	C2-N1-C1'	-6.88	109.45	117.70
1	1A	2729	G	C5-C6-N1	-6.88	108.06	111.50
1	2A	435	C	N1-C2-O2	6.88	123.03	118.90
1	2A	805	G	N1-C2-N3	6.88	128.03	123.90
1	1A	13	A	N1-C6-N6	-6.87	114.48	118.60
1	1A	2598	A	P-O3'-C3'	6.87	127.95	119.70
1	2A	1339	G	O5'-P-OP2	6.87	118.95	110.70
32	2a	446	G	C8-N9-C4	-6.87	103.65	106.40
1	1A	29	U	O5'-P-OP2	-6.87	99.52	105.70
1	1A	782	A	C6-N1-C2	-6.87	114.48	118.60
1	1A	1992	G	N1-C6-O6	6.87	124.02	119.90
1	1A	2746	U	C5-C6-N1	-6.87	119.27	122.70
1	2A	2056	G	N1-C6-O6	6.87	124.02	119.90
1	1A	1250	G	C5-C6-N1	6.87	114.93	111.50
1	2A	1660	C	N3-C4-N4	-6.87	113.19	118.00
1	2A	1758	G	N1-C6-O6	6.87	124.02	119.90
1	1A	694	U	C6-N1-C2	-6.86	116.88	121.00
1	1A	2221	G	C8-N9-C4	-6.86	103.66	106.40
1	1A	2238	G	C2-N3-C4	6.86	115.33	111.90
1	1A	2414	G	C4-C5-C6	6.86	122.92	118.80
1	2A	1284	A	N1-C6-N6	6.86	122.72	118.60
1	2A	2040	C	C5-C4-N4	-6.86	115.39	120.20
1	1A	1018	C	C6-N1-C2	6.86	123.05	120.30
1	2A	1313	U	O4'-C1'-N1	6.86	113.69	108.20
1	2A	1430	C	OP1-P-OP2	6.86	129.89	119.60
1	1A	1964	G	N9-C4-C5	-6.86	102.66	105.40
1	1A	2145	C	C5-C6-N1	6.86	124.43	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1597	A	O5'-P-OP2	-6.86	99.53	105.70
32	2a	697	U	O5'-P-OP2	-6.86	99.53	105.70
1	1A	2585	U	N3-C4-O4	-6.86	114.60	119.40
1	1A	2726	U	O5'-P-OP2	-6.86	99.53	105.70
1	2A	706	A	C2-N3-C4	-6.86	107.17	110.60
1	1A	19	C	N3-C4-C5	-6.86	119.16	121.90
1	1A	500	G	C5-C6-N1	-6.86	108.07	111.50
1	1A	2379	G	C4-C5-N7	6.86	113.54	110.80
1	1A	579	G	N1-C2-N2	6.85	122.37	116.20
1	1A	650	C	N3-C2-O2	-6.85	117.10	121.90
1	1A	1602	U	C5-C4-O4	6.85	130.01	125.90
1	2A	2502	G	C8-N9-C4	-6.85	103.66	106.40
2	2B	78	A	C6-N1-C2	-6.85	114.49	118.60
32	2a	1477	C	C6-N1-C2	-6.85	117.56	120.30
1	1A	2388	A	C5-C6-N6	6.85	129.18	123.70
32	1a	805	C	O5'-P-OP2	-6.85	99.54	105.70
32	1a	1466	C	C6-N1-C1'	6.85	129.02	120.80
1	2A	2607	G	N1-C6-O6	6.85	124.01	119.90
1	1A	590	A	C8-N9-C4	-6.85	103.06	105.80
32	1a	172	A	N1-C6-N6	-6.85	114.49	118.60
1	2A	1290	C	N1-C2-O2	6.85	123.01	118.90
1	2A	2547	U	O5'-P-OP1	6.85	118.92	110.70
1	1A	703	U	N1-C2-N3	-6.84	110.79	114.90
1	1A	763	G	N1-C2-N3	6.84	128.01	123.90
1	1A	969	U	C5-C6-N1	-6.84	119.28	122.70
1	2A	784	A	N9-C4-C5	6.84	108.54	105.80
32	1a	1153	C	C6-N1-C2	6.84	123.04	120.30
1	2A	2296	U	N3-C2-O2	-6.84	117.41	122.20
1	1A	1266	G	N3-C2-N2	6.84	124.69	119.90
1	1A	1327	C	N1-C2-N3	6.84	123.99	119.20
1	1A	2423	U	C5-C6-N1	-6.84	119.28	122.70
1	2A	1374	G	N1-C6-O6	6.84	124.00	119.90
1	1A	1373	A	N7-C8-N9	-6.84	110.38	113.80
1	1A	1609	A	N9-C4-C5	-6.84	103.06	105.80
1	1A	1673	U	OP2-P-O3'	6.84	120.25	105.20
1	2A	189	G	C8-N9-C4	6.84	109.14	106.40
32	2a	345	C	N3-C4-C5	-6.84	119.16	121.90
32	2a	561	U	N3-C4-O4	6.84	124.19	119.40
1	1A	2054	A	N1-C6-N6	6.84	122.70	118.60
1	1A	2818	G	N3-C4-C5	6.84	132.02	128.60
1	1A	905	U	N3-C4-O4	-6.84	114.61	119.40
1	1A	2027	G	N7-C8-N9	-6.84	109.68	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	864	G	C8-N9-C4	-6.84	103.67	106.40
1	2A	1688	U	N1-C2-N3	6.84	119.00	114.90
32	2a	922	G	O5'-P-OP1	-6.84	99.55	105.70
1	1A	458	G	C8-N9-C4	-6.83	103.67	106.40
1	1A	1663	C	C5-C4-N4	-6.83	115.42	120.20
32	1a	1505	G	C4-N9-C1'	-6.83	117.61	126.50
1	2A	1374	G	C4-C5-N7	6.83	113.53	110.80
1	2A	2220	G	N1-C6-O6	6.83	124.00	119.90
1	1A	1239	G	C5-C6-O6	-6.83	124.50	128.60
1	2A	1653	G	N1-C6-O6	6.83	124.00	119.90
1	2A	2375	G	N3-C4-C5	6.83	132.02	128.60
1	1A	1296	G	N7-C8-N9	-6.83	109.68	113.10
1	1A	1396	U	O5'-P-OP1	-6.83	99.55	105.70
1	1A	1759	A	O5'-P-OP1	-6.83	99.55	105.70
1	1A	1970	A	O4'-C1'-N9	-6.83	102.73	108.20
1	1A	2464	C	N1-C2-O2	-6.83	114.80	118.90
1	2A	855	G	C8-N9-C4	-6.83	103.67	106.40
1	1A	78	A	N1-C6-N6	6.83	122.70	118.60
1	1A	920	G	C5-C6-N1	-6.83	108.09	111.50
1	1A	1302	A	O5'-P-OP2	-6.83	99.55	105.70
1	1A	1367	A	N1-C2-N3	6.83	132.71	129.30
1	1A	1604	C	N3-C4-N4	6.83	122.78	118.00
1	1A	1982	C	C6-N1-C2	-6.83	117.57	120.30
1	1A	2650	U	N3-C4-O4	-6.83	114.62	119.40
1	2A	2078	C	N3-C4-C5	-6.83	119.17	121.90
32	1a	781	A	C5-N7-C8	-6.83	100.49	103.90
1	2A	2017	U	N1-C2-N3	6.83	119.00	114.90
32	2a	421	U	N1-C2-O2	6.83	127.58	122.80
1	1A	1217	C	C5-C4-N4	-6.83	115.42	120.20
1	1A	2003	G	C5-C6-O6	-6.82	124.51	128.60
1	1A	2088	G	C2-N3-C4	-6.82	108.49	111.90
1	1A	272(E)	G	N9-C4-C5	-6.82	102.67	105.40
1	1A	2584	U	C6-N1-C2	-6.82	116.91	121.00
32	1a	758	G	N1-C6-O6	6.82	123.99	119.90
46	1o	67	LEU	CA-CB-CG	-6.82	99.62	115.30
1	2A	508	G	N1-C6-O6	6.82	123.99	119.90
1	2A	2804	C	C6-N1-C2	-6.82	117.57	120.30
1	1A	399	G	C5-C6-O6	-6.82	124.51	128.60
1	1A	510	C	O5'-P-OP2	-6.82	99.57	105.70
1	1A	2022	U	C5-C4-O4	-6.82	121.81	125.90
32	1a	615	C	C5-C6-N1	6.82	124.41	121.00
32	1a	1417	G	N1-C6-O6	-6.82	115.81	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	687	C	N1-C2-N3	6.82	123.97	119.20
32	2a	1397	C	C6-N1-C1'	-6.82	112.62	120.80
32	1a	327	A	N1-C6-N6	6.81	122.69	118.60
32	1a	1151	A	C8-N9-C4	-6.81	103.08	105.80
1	2A	1904	G	C8-N9-C4	6.81	109.12	106.40
1	2A	1265	A	C8-N9-C4	6.81	108.52	105.80
1	1A	121	G	C5-C6-O6	-6.81	124.51	128.60
1	1A	1014	U	N3-C4-C5	-6.81	110.52	114.60
1	1A	2019	A	N1-C6-N6	6.81	122.69	118.60
1	2A	1973	G	N1-C2-N2	-6.81	110.07	116.20
1	2A	2573	C	C5-C6-N1	6.81	124.40	121.00
1	1A	272(E)	G	C4-C5-N7	6.81	113.52	110.80
1	1A	481	G	O4'-C1'-N9	6.81	113.65	108.20
1	1A	1380	G	O5'-P-OP2	-6.81	99.57	105.70
1	1A	100	G	OP1-P-OP2	6.80	129.81	119.60
1	1A	236	C	C5-C6-N1	-6.80	117.60	121.00
1	1A	476	G	C8-N9-C4	6.80	109.12	106.40
1	1A	987	G	OP1-P-O3'	6.80	120.17	105.20
1	1A	2562	U	N1-C2-N3	6.80	118.98	114.90
1	2A	2652	C	C6-N1-C2	6.80	123.02	120.30
1	1A	2715	C	C5-C6-N1	-6.80	117.60	121.00
1	1A	1983	C	C4-C5-C6	6.80	120.80	117.40
32	1a	1436	U	C2-N3-C4	-6.80	122.92	127.00
1	1A	508	G	C4-N9-C1'	-6.80	117.66	126.50
1	1A	2711	A	N3-C4-C5	6.80	131.56	126.80
1	2A	2877	G	C8-N9-C4	6.80	109.12	106.40
1	1A	1758	G	N3-C4-N9	-6.79	121.92	126.00
32	1a	705	U	C6-N1-C2	-6.79	116.92	121.00
32	1a	1183	A	OP1-P-O3'	6.79	120.15	105.20
1	2A	257	A	N1-C6-N6	-6.79	114.52	118.60
1	1A	442	G	N7-C8-N9	6.79	116.50	113.10
1	1A	1338	G	OP1-P-OP2	-6.79	109.41	119.60
1	1A	2582	G	O5'-P-OP1	-6.79	99.59	105.70
1	1A	2801(A)	A	C8-N9-C4	-6.79	103.08	105.80
1	1A	842	G	N3-C4-C5	6.79	132.00	128.60
1	1A	1821	A	C2-N3-C4	-6.79	107.20	110.60
32	1a	339	C	C5-C6-N1	-6.79	117.60	121.00
1	2A	936	C	C6-N1-C2	6.79	123.02	120.30
1	1A	913	U	C5-C4-O4	6.79	129.97	125.90
32	2a	244	U	N1-C2-N3	-6.79	110.83	114.90
32	2a	776	G	C2-N3-C4	-6.79	108.50	111.90
1	1A	488	G	N1-C6-O6	-6.79	115.83	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1257	C	N3-C2-O2	-6.79	117.15	121.90
1	1A	2452	C	N3-C4-C5	6.79	124.61	121.90
32	1a	481	G	C8-N9-C1'	-6.79	118.17	127.00
1	2A	1686	C	N3-C2-O2	-6.79	117.15	121.90
1	2A	1287	A	N1-C6-N6	6.79	122.67	118.60
1	1A	21	A	OP1-P-O3'	6.79	120.13	105.20
1	1A	1814	G	N3-C4-N9	-6.79	121.93	126.00
1	1A	1823	G	OP1-P-OP2	-6.79	109.42	119.60
1	1A	1969	A	N1-C2-N3	6.79	132.69	129.30
1	2A	2586	C	C6-N1-C2	6.79	123.01	120.30
1	2A	2751	G	C5-C6-O6	6.78	132.67	128.60
32	1a	1523	G	N9-C4-C5	6.78	108.11	105.40
1	2A	1401	G	C8-N9-C4	-6.78	103.69	106.40
1	2A	2205	C	C6-N1-C2	-6.78	117.59	120.30
1	1A	1517	G	N1-C6-O6	6.78	123.97	119.90
1	1A	2685	G	C4-C5-N7	-6.78	108.09	110.80
1	2A	741	G	N1-C6-O6	-6.78	115.83	119.90
1	1A	12	U	C2-N1-C1'	6.78	125.83	117.70
1	1A	648	G	C2-N3-C4	-6.78	108.51	111.90
1	1A	688	U	N1-C2-O2	-6.78	118.06	122.80
1	1A	985	C	C6-N1-C2	-6.78	117.59	120.30
1	1A	2714	G	O5'-P-OP2	-6.78	99.60	105.70
1	2A	1673	U	O5'-P-OP2	6.78	118.83	110.70
32	2a	1061	G	C8-N9-C4	-6.78	103.69	106.40
1	1A	2463	C	N1-C2-O2	-6.77	114.84	118.90
1	2A	528	A	C8-N9-C4	-6.77	103.09	105.80
1	1A	1395	A	C8-N9-C4	6.77	108.51	105.80
1	1A	1553	A	O5'-P-OP2	6.77	118.83	110.70
1	1A	2022	U	C2-N3-C4	-6.77	122.94	127.00
32	1a	818	G	C8-N9-C4	-6.77	103.69	106.40
1	2A	2437	U	N3-C2-O2	6.77	126.94	122.20
1	2A	2179	C	C5-C6-N1	6.77	124.39	121.00
32	2a	1436	U	C5-C4-O4	-6.77	121.84	125.90
1	1A	227	A	C6-N1-C2	-6.77	114.54	118.60
1	1A	1506	C	C6-N1-C2	-6.77	117.59	120.30
1	1A	1654	A	C8-N9-C4	-6.77	103.09	105.80
1	1A	2782	G	C5-C6-O6	-6.77	124.54	128.60
1	1A	358	U	O5'-P-OP1	-6.77	99.61	105.70
32	1a	266	G	O4'-C1'-N9	-6.77	102.79	108.20
32	1a	728	A	C8-N9-C4	-6.77	103.09	105.80
1	2A	1146	C	N3-C4-C5	-6.77	119.19	121.90
1	2A	1382	G	N3-C4-C5	6.77	131.98	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	264	U	C2-N1-C1'	6.77	125.82	117.70
1	1A	448	U	C5-C4-O4	6.77	129.96	125.90
1	1A	2520	C	N1-C2-O2	-6.77	114.84	118.90
1	1A	19	C	OP1-P-OP2	-6.76	109.45	119.60
1	1A	1137	G	N7-C8-N9	6.76	116.48	113.10
1	1A	2555	U	N3-C2-O2	6.76	126.94	122.20
1	1A	2740	A	C4-C5-C6	6.76	120.38	117.00
1	2A	1293	C	N3-C2-O2	6.76	126.64	121.90
1	2A	1321	A	C2-N3-C4	-6.76	107.22	110.60
1	2A	1653	G	C6-C5-N7	-6.76	126.34	130.40
1	2A	2284	C	C6-N1-C2	6.76	123.01	120.30
1	1A	2068	U	C2-N3-C4	-6.76	122.94	127.00
1	1A	2362	G	O5'-P-OP1	-6.76	99.61	105.70
1	1A	2550	G	N9-C4-C5	6.76	108.11	105.40
1	2A	1372	U	N3-C4-O4	6.76	124.13	119.40
32	2a	1119	C	C6-N1-C2	-6.76	117.59	120.30
1	1A	1283	G	N3-C2-N2	6.76	124.63	119.90
32	1a	27	G	O5'-P-OP1	-6.76	99.62	105.70
32	1a	1397	C	C6-N1-C2	-6.76	117.60	120.30
1	2A	1686	C	C4-C5-C6	6.76	120.78	117.40
1	2A	2102	U	C2-N1-C1'	6.76	125.81	117.70
1	1A	2447	G	N1-C6-O6	6.76	123.95	119.90
1	1A	485	C	C6-N1-C2	6.76	123.00	120.30
1	2A	1248	G	O5'-P-OP1	6.76	118.81	110.70
1	2A	1661	G	C5-C6-O6	-6.76	124.55	128.60
1	2A	2288	A	N9-C4-C5	-6.76	103.10	105.80
1	1A	1701	A	C5-C6-N6	-6.75	118.30	123.70
1	1A	2562	U	C4-C5-C6	6.75	123.75	119.70
2	2B	15	A	C8-N9-C4	6.75	108.50	105.80
32	2a	244	U	C6-N1-C1'	-6.75	111.74	121.20
32	2a	730	G	N9-C4-C5	6.75	108.10	105.40
1	1A	624	C	N3-C4-C5	6.75	124.60	121.90
32	1a	1516	G	N3-C4-N9	-6.75	121.95	126.00
1	2A	614(C)	A	C8-N9-C4	-6.75	103.10	105.80
1	1A	1613	G	C5-C6-O6	6.75	132.65	128.60
1	1A	2091	U	C5-C6-N1	-6.75	119.33	122.70
1	2A	2347	C	O5'-P-OP2	-6.75	99.62	105.70
1	1A	122	G	N9-C4-C5	-6.75	102.70	105.40
1	1A	584	C	OP1-P-O3'	6.75	120.05	105.20
1	1A	745	G	C5-C6-O6	-6.75	124.55	128.60
1	1A	1701	A	N1-C6-N6	6.75	122.65	118.60
1	1A	2511	U	N1-C2-N3	6.75	118.95	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1259	C	C5-C6-N1	6.75	124.38	121.00
1	1A	2524	G	O5'-P-OP2	-6.75	99.63	105.70
2	1B	32	C	N3-C4-N4	-6.75	113.28	118.00
1	2A	1372	U	C2-N1-C1'	6.75	125.80	117.70
2	1B	96	U	C5-C4-O4	6.75	129.95	125.90
1	2A	1647	G	C8-N9-C4	6.75	109.10	106.40
1	1A	1284	A	C5-C6-N6	-6.74	118.31	123.70
1	1A	2451	A	N7-C8-N9	6.74	117.17	113.80
1	2A	2088	G	C2-N3-C4	-6.74	108.53	111.90
1	1A	329	G	N9-C4-C5	-6.74	102.70	105.40
1	1A	470	A	C6-N1-C2	-6.74	114.56	118.60
1	1A	1824	G	C8-N9-C4	6.74	109.10	106.40
1	2A	749	C	C2-N3-C4	6.74	123.27	119.90
1	1A	758	C	O5'-P-OP1	6.74	118.79	110.70
1	1A	1054	A	C8-N9-C4	-6.74	103.10	105.80
1	2A	606	U	N3-C4-O4	-6.74	114.68	119.40
1	2A	702	G	O5'-P-OP2	-6.74	99.64	105.70
1	2A	812	C	C4-C5-C6	6.74	120.77	117.40
1	2A	2615	U	N3-C4-C5	6.74	118.64	114.60
2	2B	59	A	C6-N1-C2	-6.74	114.56	118.60
1	1A	1184	G	C2-N3-C4	-6.74	108.53	111.90
32	1a	404	U	C2-N1-C1'	6.74	125.78	117.70
1	2A	1560	G	C8-N9-C4	6.74	109.09	106.40
1	1A	932	G	C5-C6-O6	6.74	132.64	128.60
1	2A	563	G	C5-N7-C8	-6.74	100.93	104.30
1	2A	2241	A	N1-C6-N6	-6.74	114.56	118.60
32	2a	30	U	O5'-P-OP2	-6.74	99.64	105.70
1	1A	949	C	N1-C2-O2	-6.73	114.86	118.90
1	1A	236	C	N1-C2-N3	6.73	123.91	119.20
1	1A	1193	G	O5'-P-OP2	-6.73	99.64	105.70
1	1A	2399	G	C2-N3-C4	6.73	115.27	111.90
32	2a	1054	C	C2-N1-C1'	6.73	126.21	118.80
1	1A	441	U	N3-C4-C5	6.73	118.64	114.60
1	1A	1342	A	C5-C6-N6	-6.73	118.32	123.70
17	1V	83	ARG	NE-CZ-NH2	6.73	123.67	120.30
1	2A	1159	U	C5-C6-N1	-6.73	119.33	122.70
1	1A	227	A	N3-C4-C5	-6.73	122.09	126.80
1	1A	856	C	N3-C4-C5	-6.73	119.21	121.90
1	1A	669	G	C6-C5-N7	-6.73	126.36	130.40
1	1A	1162	G	C6-C5-N7	6.73	134.44	130.40
1	1A	192	C	N1-C2-O2	-6.72	114.86	118.90
1	1A	751	A	N1-C2-N3	6.72	132.66	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1853	A	N1-C6-N6	-6.72	114.56	118.60
32	1a	911	U	C4-C5-C6	6.72	123.73	119.70
1	1A	2504	U	N1-C2-N3	-6.72	110.87	114.90
1	2A	1364	G	N1-C6-O6	-6.72	115.87	119.90
2	1B	47	C	N3-C2-O2	6.72	126.61	121.90
1	2A	718	A	C6-C5-N7	-6.72	127.59	132.30
1	1A	194	G	N3-C4-C5	6.72	131.96	128.60
1	1A	967	C	C4-C5-C6	6.72	120.76	117.40
1	1A	1645	G	N3-C4-C5	-6.72	125.24	128.60
1	1A	2741	A	O5'-P-OP2	-6.72	99.65	105.70
1	1A	2747	G	N1-C6-O6	6.72	123.93	119.90
2	1B	57	A	OP1-P-OP2	-6.72	109.52	119.60
1	2A	822	U	C6-N1-C2	-6.72	116.97	121.00
1	2A	1416	G	O4'-C1'-N9	6.72	113.58	108.20
1	1A	390	A	N9-C4-C5	-6.72	103.11	105.80
1	1A	1672	C	N3-C4-N4	6.72	122.70	118.00
1	1A	2699	C	N3-C4-N4	6.72	122.70	118.00
32	1a	1397	C	C5-C6-N1	6.72	124.36	121.00
1	2A	570	G	N1-C6-O6	-6.72	115.87	119.90
1	2A	1396	U	O5'-P-OP1	-6.72	99.66	105.70
1	2A	1415	U	C5-C4-O4	6.72	129.93	125.90
1	2A	2133	G	C8-N9-C4	6.72	109.09	106.40
1	1A	1753	G	C2-N3-C4	-6.71	108.54	111.90
1	1A	2394	C	C2-N3-C4	-6.71	116.54	119.90
1	2A	2801(A)	A	C8-N9-C4	-6.71	103.11	105.80
1	1A	494	G	C8-N9-C4	-6.71	103.72	106.40
32	1a	783	C	C5-C4-N4	6.71	124.90	120.20
1	1A	739	G	C5-C6-O6	-6.71	124.57	128.60
1	1A	1889	A	C8-N9-C4	6.71	108.48	105.80
1	1A	2052	G	C4-C5-N7	6.71	113.48	110.80
32	1a	73	G	C4-N9-C1'	-6.71	117.78	126.50
32	1a	800	G	O5'-P-OP2	-6.71	99.66	105.70
32	1a	1415	G	C4-C5-N7	6.71	113.48	110.80
1	2A	391	G	N3-C4-N9	6.71	130.03	126.00
1	1A	12	U	C6-N1-C2	-6.71	116.97	121.00
1	1A	569	U	OP1-P-OP2	6.71	129.66	119.60
1	2A	1525	G	OP1-P-OP2	6.71	129.66	119.60
1	2A	2761	G	C8-N9-C4	-6.71	103.72	106.40
1	1A	974	G	C8-N9-C4	-6.71	103.72	106.40
1	1A	2598	A	C8-N9-C4	-6.71	103.12	105.80
1	1A	2770	G	N3-C4-C5	-6.71	125.25	128.60
1	2A	252	G	C4-C5-N7	-6.71	108.12	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1981	A	C5-N7-C8	-6.71	100.55	103.90
1	1A	205	G	N9-C4-C5	-6.71	102.72	105.40
1	1A	1295	C	C2-N3-C4	-6.71	116.55	119.90
32	2a	926	G	N3-C4-C5	-6.71	125.25	128.60
1	2A	2677	G	C6-C5-N7	-6.70	126.38	130.40
32	2a	398	C	N3-C4-N4	-6.70	113.31	118.00
1	1A	446	G	C5-C6-O6	-6.70	124.58	128.60
1	2A	2560	C	C6-N1-C2	6.70	122.98	120.30
1	1A	1786	A	C8-N9-C4	6.70	108.48	105.80
1	1A	2782	G	N1-C6-O6	6.70	123.92	119.90
1	1A	325	G	N1-C6-O6	6.70	123.92	119.90
1	1A	982	C	C5-C6-N1	6.70	124.35	121.00
1	1A	1277	G	C8-N9-C4	6.70	109.08	106.40
1	1A	2609	U	C2-N3-C4	-6.70	122.98	127.00
32	1a	660	G	C6-C5-N7	-6.70	126.38	130.40
1	2A	2060	A	N1-C6-N6	-6.70	114.58	118.60
1	1A	1096	A	N1-C6-N6	-6.70	114.58	118.60
1	2A	1188	U	N3-C4-O4	-6.70	114.71	119.40
1	1A	761	A	C5-N7-C8	6.70	107.25	103.90
1	1A	2534	A	C5-C6-N1	6.70	121.05	117.70
1	2A	932	G	N3-C4-C5	6.70	131.95	128.60
1	2A	2858	C	C6-N1-C2	6.70	122.98	120.30
1	1A	1657	C	C2-N1-C1'	-6.69	111.44	118.80
1	1A	2068	U	N1-C2-N3	6.69	118.92	114.90
1	2A	1076	C	N3-C4-C5	-6.69	119.22	121.90
1	1A	1216	G	N1-C2-N3	6.69	127.92	123.90
1	1A	1678	G	C8-N9-C4	-6.69	103.72	106.40
1	1A	1787	A	N1-C6-N6	6.69	122.61	118.60
1	1A	2550	G	N3-C4-C5	-6.69	125.25	128.60
1	1A	2588	G	C5-C6-O6	6.69	132.62	128.60
1	2A	2463	C	N3-C2-O2	6.69	126.58	121.90
1	2A	2755	C	C2-N1-C1'	6.69	126.16	118.80
1	1A	785	G	N9-C4-C5	6.69	108.08	105.40
1	1A	993	G	C6-C5-N7	6.69	134.41	130.40
1	1A	2393	A	N1-C6-N6	-6.69	114.59	118.60
32	2a	360	A	O5'-P-OP2	-6.69	99.68	105.70
1	2A	2511	U	N1-C2-N3	6.69	118.91	114.90
1	1A	1763	G	OP2-P-O3'	6.69	119.91	105.20
1	2A	572	A	N7-C8-N9	6.69	117.14	113.80
1	1A	1274	A	C5-C6-N1	-6.68	114.36	117.70
1	1A	1656	C	C5-C6-N1	6.68	124.34	121.00
2	1B	41	U	C2-N1-C1'	-6.68	109.68	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1516	G	N3-C4-C5	6.68	131.94	128.60
1	1A	2445	G	C5-C6-O6	6.68	132.61	128.60
1	1A	200	U	C6-N1-C2	-6.68	116.99	121.00
1	1A	1853	A	C5-C6-N6	6.68	129.04	123.70
1	2A	679	C	N3-C2-O2	6.68	126.58	121.90
32	2a	421	U	C2-N1-C1'	6.68	125.72	117.70
1	1A	372	G	N1-C6-O6	6.68	123.91	119.90
32	1a	119	A	C8-N9-C4	6.68	108.47	105.80
1	2A	123	G	N1-C2-N3	6.68	127.91	123.90
1	2A	574	C	C6-N1-C2	6.68	122.97	120.30
1	2A	1068	G	O4'-C1'-N9	6.68	113.54	108.20
1	2A	1340	U	C2-N3-C4	-6.68	122.99	127.00
1	2A	2413	G	C8-N9-C4	6.68	109.07	106.40
1	2A	2896	C	C6-N1-C2	-6.68	117.63	120.30
32	1a	1192	C	C5-C6-N1	6.68	124.34	121.00
32	2a	79	G	C8-N9-C4	-6.68	103.73	106.40
1	1A	739	G	C4-C5-N7	6.68	113.47	110.80
1	1A	2553	G	N3-C4-N9	6.68	130.01	126.00
2	1B	4	C	C6-N1-C2	6.67	122.97	120.30
5	2F	196	LEU	CA-CB-CG	-6.67	99.95	115.30
1	1A	803	U	C5-C6-N1	-6.67	119.36	122.70
1	1A	1025	G	C2-N3-C4	-6.67	108.56	111.90
32	1a	1474	G	C8-N9-C4	6.67	109.07	106.40
1	2A	883	G	C8-N9-C4	6.67	109.07	106.40
1	2A	1783	A	C8-N9-C4	-6.67	103.13	105.80
1	2A	2579	C	N1-C2-N3	-6.67	114.53	119.20
1	1A	1456	G	N1-C6-O6	6.67	123.90	119.90
1	2A	834	C	N3-C2-O2	-6.67	117.23	121.90
32	2a	1285	A	P-O3'-C3'	6.67	127.70	119.70
1	1A	1222	C	N3-C2-O2	6.67	126.57	121.90
1	1A	2714	G	C5-C6-O6	-6.67	124.60	128.60
1	2A	2523	G	N1-C6-O6	6.67	123.90	119.90
1	1A	2031	A	C2-N3-C4	6.67	113.93	110.60
1	2A	2705	A	C2-N3-C4	-6.67	107.27	110.60
1	2A	555	U	O5'-P-OP2	-6.66	99.70	105.70
32	2a	841	U	N1-C2-O2	6.66	127.47	122.80
32	2a	898	G	C4-C5-N7	6.66	113.47	110.80
1	1A	623	G	C8-N9-C4	6.66	109.06	106.40
32	1a	1030	C	C5-C6-N1	6.66	124.33	121.00
1	1A	74	A	O5'-P-OP1	6.66	118.69	110.70
1	1A	2036	C	C5-C6-N1	-6.66	117.67	121.00
1	1A	2371	G	N7-C8-N9	-6.66	109.77	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2061	G	N1-C6-O6	6.66	123.90	119.90
32	2a	1499	A	O5'-P-OP1	6.66	118.69	110.70
1	1A	1625	C	C5-C4-N4	6.66	124.86	120.20
1	1A	1834	U	O5'-P-OP1	-6.66	99.71	105.70
32	1a	618	C	C5-C6-N1	6.66	124.33	121.00
32	1a	965	A	C4-C5-C6	-6.66	113.67	117.00
1	2A	863	A	N1-C6-N6	6.66	122.59	118.60
1	2A	1230	C	O5'-P-OP1	6.66	118.69	110.70
1	2A	2088	G	N1-C6-O6	6.66	123.90	119.90
1	2A	2231	C	C4-C5-C6	6.66	120.73	117.40
32	2a	230	G	C8-N9-C4	-6.66	103.74	106.40
32	1a	977	A	O5'-P-OP2	-6.66	99.71	105.70
1	1A	502	A	O5'-P-OP2	6.66	118.69	110.70
1	1A	620	G	O5'-P-OP1	-6.66	99.71	105.70
1	1A	2446	G	O5'-P-OP2	-6.66	99.71	105.70
32	1a	893	C	C6-N1-C1'	-6.66	112.81	120.80
1	2A	2267	A	C6-C5-N7	-6.66	127.64	132.30
1	1A	1831	G	C5-C6-N1	-6.65	108.17	111.50
1	1A	197	A	N1-C6-N6	6.65	122.59	118.60
1	1A	1156	A	C8-N9-C4	-6.65	103.14	105.80
1	1A	2060	A	N1-C6-N6	-6.65	114.61	118.60
1	1A	2491	U	N3-C2-O2	6.65	126.86	122.20
1	2A	852	G	O5'-P-OP1	6.65	118.68	110.70
1	1A	1936	A	O5'-P-OP2	6.65	118.68	110.70
1	2A	294	A	N1-C6-N6	-6.65	114.61	118.60
1	2A	713	G	C2-N3-C4	-6.65	108.57	111.90
1	2A	2180	U	C5-C6-N1	6.65	126.03	122.70
32	2a	687	A	P-O3'-C3'	6.65	127.68	119.70
1	1A	641	C	OP2-P-O3'	6.65	119.83	105.20
1	1A	2294	C	N3-C2-O2	-6.65	117.25	121.90
1	2A	1022	G	N9-C4-C5	6.65	108.06	105.40
1	1A	209	C	C6-N1-C2	6.65	122.96	120.30
32	1a	1028	C	C6-N1-C2	-6.65	117.64	120.30
1	2A	171	G	N3-C4-C5	-6.65	125.28	128.60
1	2A	365	C	C6-N1-C2	-6.65	117.64	120.30
1	2A	330	A	C2-N3-C4	-6.65	107.28	110.60
1	2A	960	A	N1-C6-N6	6.65	122.59	118.60
32	2a	800	G	OP2-P-O3'	6.65	119.82	105.20
2	1B	79	C	N3-C4-N4	-6.64	113.35	118.00
1	2A	966	G	C8-N9-C4	-6.64	103.74	106.40
2	2B	79	C	N3-C4-C5	-6.64	119.24	121.90
1	1A	189	G	C6-C5-N7	-6.64	126.42	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	271	A	N1-C6-N6	6.64	122.58	118.60
1	1A	2568	C	N3-C4-C5	-6.64	119.24	121.90
1	2A	1231	G	C5-C6-N1	-6.64	108.18	111.50
16	1U	55	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	1A	40	C	O5'-P-OP1	6.64	118.67	110.70
1	1A	812	C	N1-C2-O2	-6.64	114.92	118.90
1	2A	198	C	O5'-P-OP2	-6.64	99.72	105.70
1	2A	1254	A	C6-N1-C2	-6.64	114.62	118.60
1	1A	443	A	O5'-P-OP2	-6.64	99.73	105.70
1	1A	434	U	N1-C2-O2	-6.64	118.15	122.80
1	1A	703	U	N3-C2-O2	6.64	126.85	122.20
1	1A	2033	A	O4'-C1'-N9	6.64	113.51	108.20
2	1B	101	G	N1-C2-N3	6.64	127.88	123.90
1	2A	329	G	C5-C6-O6	-6.64	124.62	128.60
1	2A	778	G	C8-N9-C4	6.64	109.05	106.40
1	2A	794	G	C5-C6-N1	-6.64	108.18	111.50
2	2B	117	G	N3-C4-C5	6.64	131.92	128.60
1	1A	761	A	N7-C8-N9	-6.63	110.48	113.80
1	1A	1780	A	N7-C8-N9	6.63	117.12	113.80
1	2A	213	A	N7-C8-N9	-6.63	110.48	113.80
1	2A	1365	A	C4-C5-N7	-6.63	107.38	110.70
1	2A	1270	C	C5-C4-N4	6.63	124.84	120.20
1	2A	1618	A	C8-N9-C4	-6.63	103.15	105.80
1	1A	843	G	C8-N9-C4	6.63	109.05	106.40
1	1A	1395	A	C5-N7-C8	6.63	107.22	103.90
32	1a	722	A	C5-N7-C8	-6.63	100.58	103.90
1	2A	818	G	C2-N3-C4	-6.63	108.58	111.90
1	2A	1583	A	N1-C6-N6	-6.63	114.62	118.60
1	2A	2606	C	C2-N1-C1'	-6.63	111.51	118.80
1	1A	28	A	N1-C6-N6	6.63	122.58	118.60
1	1A	981	A	N1-C2-N3	-6.63	125.99	129.30
1	1A	1989	G	C4-C5-N7	6.63	113.45	110.80
32	1a	624	C	C6-N1-C2	-6.63	117.65	120.30
32	2a	801	U	C5-C4-O4	-6.63	121.92	125.90
1	1A	394	A	N1-C6-N6	-6.63	114.62	118.60
1	1A	1183	G	N1-C6-O6	-6.63	115.92	119.90
1	1A	1647	G	O4'-C1'-N9	-6.63	102.90	108.20
1	2A	1187	G	O5'-P-OP2	-6.63	99.74	105.70
1	2A	2365	G	N3-C4-N9	6.63	129.98	126.00
32	2a	1403	C	O5'-P-OP2	-6.63	99.74	105.70
1	1A	918	A	O5'-P-OP1	-6.62	99.74	105.70
1	1A	2624	G	C2-N3-C4	-6.62	108.59	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2850	A	C5-C6-N6	-6.62	118.40	123.70
1	2A	1542	A	C8-N9-C4	-6.62	103.15	105.80
1	1A	1405	U	O5'-P-OP2	-6.62	99.74	105.70
1	2A	679	C	N1-C2-O2	-6.62	114.93	118.90
1	2A	1430	C	C6-N1-C2	-6.62	117.65	120.30
32	2a	301	G	O5'-P-OP1	6.62	118.65	110.70
1	2A	271(W)	G	C5-C6-N1	-6.62	108.19	111.50
32	2a	1067	A	C2-N3-C4	6.62	113.91	110.60
1	1A	2431	U	N1-C2-N3	6.62	118.87	114.90
1	1A	880	G	C8-N9-C4	-6.62	103.75	106.40
1	1A	110	G	C8-N9-C4	6.62	109.05	106.40
1	1A	267	C	C4-C5-C6	-6.62	114.09	117.40
1	1A	679	C	N3-C4-C5	6.62	124.55	121.90
1	1A	1195	G	N1-C2-N2	6.62	122.15	116.20
1	1A	1263	U	O5'-P-OP2	-6.62	99.75	105.70
1	2A	994	C	N3-C2-O2	-6.62	117.27	121.90
1	1A	1762	A	C5-N7-C8	6.61	107.21	103.90
1	1A	2074	U	C5-C6-N1	6.61	126.01	122.70
1	2A	468	G	OP1-P-OP2	-6.61	109.68	119.60
1	2A	1016	G	C8-N9-C4	6.61	109.05	106.40
1	2A	2331	G	N9-C4-C5	-6.61	102.75	105.40
32	2a	730	G	C5-C6-O6	6.61	132.57	128.60
1	1A	1651	G	C6-C5-N7	-6.61	126.43	130.40
2	1B	50	G	O5'-P-OP1	6.61	118.63	110.70
32	2a	792	A	O4'-C1'-N9	6.61	113.49	108.20
32	1a	1151	A	N9-C4-C5	6.61	108.44	105.80
1	2A	2270	G	N1-C6-O6	-6.61	115.94	119.90
1	2A	2390	U	N3-C2-O2	-6.61	117.58	122.20
1	1A	398	G	N7-C8-N9	-6.61	109.80	113.10
1	1A	1433	U	O5'-P-OP2	-6.61	99.76	105.70
1	2A	592	G	N9-C4-C5	6.61	108.04	105.40
1	2A	941	A	O5'-P-OP1	-6.61	99.75	105.70
1	1A	1118	C	C6-N1-C2	6.60	122.94	120.30
4	1E	47	VAL	CB-CA-C	-6.60	98.86	111.40
1	2A	909	A	N9-C4-C5	6.60	108.44	105.80
1	2A	2518	A	OP2-P-O3'	6.60	119.72	105.20
1	1A	2784	C	C5-C4-N4	-6.60	115.58	120.20
1	2A	1495	A	C8-N9-C4	6.60	108.44	105.80
1	1A	573	G	N7-C8-N9	6.60	116.40	113.10
1	1A	1048	A	O5'-P-OP1	-6.60	99.76	105.70
1	1A	2449	U	N3-C4-O4	6.60	124.02	119.40
1	2A	2057	A	OP1-P-O3'	6.60	119.72	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	732	C	N3-C2-O2	6.60	126.52	121.90
1	2A	84	A	C8-N9-C4	6.60	108.44	105.80
1	1A	675	A	O5'-P-OP1	-6.60	99.76	105.70
1	1A	1201	C	C6-N1-C2	6.60	122.94	120.30
1	1A	2582	G	N7-C8-N9	6.60	116.40	113.10
1	1A	2285	C	O5'-P-OP2	-6.59	99.77	105.70
32	1a	1112	C	C5-C6-N1	6.59	124.30	121.00
1	2A	1415	U	N1-C2-N3	6.59	118.86	114.90
1	1A	925	C	C2-N1-C1'	-6.59	111.55	118.80
1	1A	2431	U	N3-C4-O4	-6.59	114.78	119.40
1	2A	2829	C	C6-N1-C2	6.59	122.94	120.30
1	1A	718	A	N1-C6-N6	6.59	122.56	118.60
1	1A	1993	U	C4-C5-C6	6.59	123.66	119.70
1	1A	2661	G	N1-C6-O6	-6.59	115.94	119.90
32	1a	576	G	C6-C5-N7	-6.59	126.44	130.40
1	2A	83	G	O5'-P-OP2	-6.59	99.77	105.70
1	2A	55	G	N7-C8-N9	6.59	116.39	113.10
1	2A	1312	U	N1-C2-N3	6.59	118.85	114.90
1	1A	712	G	N9-C4-C5	-6.59	102.77	105.40
32	2a	728	A	C5-C6-N6	-6.59	118.43	123.70
1	1A	2696	U	C2-N1-C1'	6.59	125.60	117.70
1	2A	1815	A	N9-C4-C5	6.59	108.43	105.80
32	2a	587	G	C8-N9-C4	-6.59	103.77	106.40
1	1A	1197	G	C5-C6-O6	-6.58	124.65	128.60
1	1A	2378	A	O4'-C1'-N9	-6.58	102.93	108.20
1	1A	2558	C	N1-C2-O2	-6.58	114.95	118.90
32	1a	625	G	C8-N9-C4	-6.58	103.77	106.40
1	1A	958	U	N3-C2-O2	6.58	126.81	122.20
1	1A	975(A)	G	N1-C2-N2	6.58	122.13	116.20
1	1A	1258	C	C6-N1-C2	6.58	122.93	120.30
1	1A	2252	G	N1-C2-N2	-6.58	110.28	116.20
1	1A	2372	G	C8-N9-C4	6.58	109.03	106.40
1	2A	2572	A	N1-C6-N6	-6.58	114.65	118.60
1	1A	763	G	N3-C4-C5	6.58	131.89	128.60
32	1a	283	C	N1-C2-O2	6.58	122.85	118.90
1	2A	2105	C	C5-C6-N1	6.58	124.29	121.00
32	1a	141	A	C8-N9-C4	-6.58	103.17	105.80
32	2a	13	U	C6-N1-C2	6.58	124.95	121.00
1	1A	1186	G	N9-C4-C5	-6.58	102.77	105.40
1	1A	1930	G	O5'-P-OP2	-6.58	99.78	105.70
1	1A	2678	C	C5-C4-N4	6.58	124.81	120.20
1	2A	1805	U	N1-C2-N3	6.58	118.85	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	333	G	O5'-P-OP2	-6.58	99.78	105.70
1	1A	446	G	C4-C5-N7	6.57	113.43	110.80
1	2A	2168	G	C8-N9-C4	-6.57	103.77	106.40
1	1A	823	G	N3-C2-N2	-6.57	115.30	119.90
1	2A	1325	G	C6-C5-N7	-6.57	126.46	130.40
1	2A	2423	U	O5'-P-OP1	-6.57	99.79	105.70
1	1A	252	G	C8-N9-C4	-6.57	103.77	106.40
1	1A	305	U	N3-C2-O2	6.57	126.80	122.20
2	1B	99	G	N9-C4-C5	-6.57	102.77	105.40
1	1A	1307	A	N7-C8-N9	-6.57	110.52	113.80
1	1A	1613	G	N1-C2-N2	-6.57	110.29	116.20
1	1A	2852	G	N9-C4-C5	-6.57	102.77	105.40
1	2A	127	A	N7-C8-N9	-6.57	110.52	113.80
1	2A	1879	C	C6-N1-C2	-6.57	117.67	120.30
1	2A	2267	A	C4-C5-C6	6.57	120.28	117.00
1	1A	195	A	OP2-P-O3'	6.57	119.64	105.20
1	1A	768	G	N3-C2-N2	-6.57	115.31	119.90
1	1A	2261	C	OP2-P-O3'	6.57	119.64	105.20
1	2A	459	U	O5'-P-OP2	-6.57	99.79	105.70
1	2A	1657	C	O5'-P-OP2	-6.57	99.79	105.70
1	2A	2008	C	C5-C6-N1	-6.57	117.72	121.00
1	2A	2556	C	N3-C2-O2	6.57	126.50	121.90
1	2A	2859	G	N3-C4-N9	6.57	129.94	126.00
32	2a	329	A	C8-N9-C4	-6.57	103.17	105.80
1	1A	2390	U	O5'-P-OP2	6.56	118.58	110.70
32	1a	181	G	N9-C4-C5	6.56	108.03	105.40
1	2A	113	G	O5'-P-OP2	-6.56	99.79	105.70
1	2A	1793	C	C5-C6-N1	-6.56	117.72	121.00
1	1A	512	G	C2-N3-C4	6.56	115.18	111.90
1	1A	1247	A	C4-C5-C6	6.56	120.28	117.00
1	1A	1627	G	N1-C6-O6	-6.56	115.96	119.90
2	1B	13	A	OP1-P-OP2	6.56	129.44	119.60
32	2a	879	C	N3-C4-N4	-6.56	113.41	118.00
1	1A	700	G	C8-N9-C4	-6.56	103.78	106.40
1	1A	1480	G	C5-C6-N1	-6.56	108.22	111.50
1	1A	1287	A	C5-C6-N6	-6.56	118.45	123.70
1	1A	1430	C	N3-C2-O2	-6.56	117.31	121.90
1	1A	2269	A	N1-C6-N6	6.56	122.54	118.60
2	1B	21	G	OP2-P-O3'	6.56	119.63	105.20
32	1a	139	G	C8-N9-C4	-6.56	103.78	106.40
32	1a	1525	G	N9-C4-C5	-6.56	102.78	105.40
1	1A	1843	C	C6-N1-C2	6.56	122.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1983	C	C5-C6-N1	-6.56	117.72	121.00
2	1B	89	G	C2-N3-C4	-6.56	108.62	111.90
1	2A	715	G	N3-C4-C5	-6.56	125.32	128.60
1	2A	2881	C	N1-C2-O2	-6.56	114.97	118.90
1	1A	2505	G	C4-C5-N7	6.56	113.42	110.80
1	2A	125	G	O5'-P-OP1	-6.56	99.80	105.70
1	1A	1277	G	C2-N3-C4	-6.55	108.62	111.90
1	1A	2230	G	O5'-P-OP1	-6.55	99.80	105.70
1	2A	947	G	N3-C4-C5	6.55	131.88	128.60
1	1A	386	G	C5-C6-O6	-6.55	124.67	128.60
1	1A	51	G	N1-C6-O6	-6.55	115.97	119.90
1	1A	2517	C	N3-C4-C5	6.55	124.52	121.90
1	1A	2730	C	C4-C5-C6	6.55	120.68	117.40
2	1B	114	C	N3-C4-C5	6.55	124.52	121.90
1	2A	575	A	O5'-P-OP2	6.55	118.56	110.70
1	2A	2488	A	C2-N3-C4	-6.55	107.33	110.60
1	1A	981	A	N9-C4-C5	-6.55	103.18	105.80
1	1A	2252	G	N3-C4-N9	6.55	129.93	126.00
1	2A	1904	G	N7-C8-N9	-6.55	109.83	113.10
32	2a	1486	G	O5'-P-OP2	-6.55	99.81	105.70
1	1A	2036	C	C2-N1-C1'	-6.54	111.60	118.80
32	1a	1113	C	C5-C6-N1	6.54	124.27	121.00
1	2A	1965	C	C6-N1-C2	6.54	122.92	120.30
1	1A	566	U	OP1-P-O3'	6.54	119.59	105.20
1	1A	1182	A	N1-C6-N6	6.54	122.53	118.60
1	2A	1297	C	N3-C4-C5	-6.54	119.28	121.90
1	2A	1497	U	N3-C2-O2	-6.54	117.62	122.20
1	1A	2447	G	N1-C2-N3	6.54	127.82	123.90
1	1A	2891	G	N1-C6-O6	6.54	123.83	119.90
2	1B	27	C	O5'-P-OP2	-6.54	99.81	105.70
1	1A	1131	G	N1-C6-O6	-6.54	115.98	119.90
32	2a	729	A	C5-N7-C8	-6.54	100.63	103.90
32	2a	893	C	N1-C2-N3	-6.54	114.62	119.20
1	1A	1651	G	C5-C6-O6	-6.54	124.68	128.60
1	1A	2837	G	N1-C6-O6	6.54	123.82	119.90
1	1A	329	G	C5-C6-O6	-6.54	124.68	128.60
1	1A	565	C	C6-N1-C2	6.54	122.91	120.30
1	1A	990	A	C5-N7-C8	-6.54	100.63	103.90
1	1A	1131	G	N1-C2-N3	-6.54	119.98	123.90
1	1A	2061	G	O5'-P-OP1	6.54	118.54	110.70
1	1A	2394	C	O5'-P-OP2	-6.54	99.82	105.70
1	2A	1257	C	C6-N1-C2	-6.54	117.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2677	G	N1-C6-O6	6.54	123.82	119.90
1	1A	325	G	N3-C4-C5	6.53	131.87	128.60
2	1B	113	G	N1-C6-O6	6.53	123.82	119.90
32	1a	738	C	C5-C6-N1	6.53	124.27	121.00
1	2A	1980	G	C5-C6-N1	6.53	114.77	111.50
1	2A	2567	G	C5-C6-O6	-6.53	124.68	128.60
1	1A	1823	G	C5-C6-N1	-6.53	108.23	111.50
1	2A	2415	G	C6-C5-N7	-6.53	126.48	130.40
1	1A	37	C	O5'-P-OP2	-6.53	99.82	105.70
1	1A	725	G	C5-C6-N1	-6.53	108.23	111.50
1	1A	2331	G	C5-C6-N1	-6.53	108.23	111.50
2	1B	98	G	N1-C6-O6	6.53	123.82	119.90
1	2A	856	C	C6-N1-C2	-6.53	117.69	120.30
1	1A	1977	A	N1-C6-N6	-6.53	114.68	118.60
1	2A	834	C	C4-C5-C6	6.53	120.66	117.40
1	2A	2441	C	C4-C5-C6	6.53	120.66	117.40
1	1A	1014	U	C6-N1-C2	-6.53	117.08	121.00
1	1A	83	G	N1-C2-N2	-6.53	110.33	116.20
1	1A	1013	C	O5'-P-OP2	-6.53	99.83	105.70
1	1A	1657	C	C5-C6-N1	-6.53	117.74	121.00
1	1A	2484	G	C6-C5-N7	-6.53	126.48	130.40
32	1a	1285	A	N1-C6-N6	-6.53	114.69	118.60
1	2A	303	U	C5-C6-N1	-6.53	119.44	122.70
1	1A	1425	G	O5'-P-OP2	-6.52	99.83	105.70
1	1A	2499	C	C2-N1-C1'	6.52	125.98	118.80
32	1a	421	U	C2-N1-C1'	6.52	125.53	117.70
1	1A	271(T)	C	C5-C6-N1	-6.52	117.74	121.00
1	1A	305	U	N3-C4-O4	6.52	123.97	119.40
1	1A	2427	C	O5'-P-OP2	6.52	118.53	110.70
8	1I	38	LEU	CA-CB-CG	6.52	130.30	115.30
1	2A	718	A	C4-C5-C6	6.52	120.26	117.00
32	1a	801	U	C2-N3-C4	-6.52	123.09	127.00
1	2A	580	C	C4-C5-C6	6.52	120.66	117.40
1	2A	888	C	P-O3'-C3'	6.52	127.53	119.70
1	1A	382	G	N7-C8-N9	-6.52	109.84	113.10
1	1A	1021	A	O5'-P-OP1	-6.52	99.83	105.70
1	1A	2278	A	N9-C4-C5	-6.52	103.19	105.80
1	2A	297	C	C6-N1-C2	-6.52	117.69	120.30
1	1A	2669	G	N1-C6-O6	6.52	123.81	119.90
32	1a	901	A	N1-C6-N6	6.52	122.51	118.60
1	2A	467	G	O5'-P-OP2	-6.52	99.83	105.70
1	1A	143	G	N3-C4-C5	6.51	131.86	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1651	G	C4-C5-N7	6.51	113.41	110.80
1	2A	452	G	N3-C2-N2	6.51	124.46	119.90
1	2A	1678	G	N3-C4-N9	6.51	129.91	126.00
1	2A	2550	G	O5'-P-OP2	-6.51	99.84	105.70
1	1A	264	C	O5'-P-OP2	-6.51	99.84	105.70
4	1E	149	ARG	NE-CZ-NH1	6.51	123.56	120.30
32	2a	380	G	C4-C5-N7	-6.51	108.19	110.80
1	1A	224	G	C5-C6-O6	6.51	132.51	128.60
1	1A	411	G	C8-N9-C4	-6.51	103.80	106.40
1	1A	796	C	C5-C6-N1	-6.51	117.74	121.00
1	1A	1409	C	OP2-P-O3'	6.51	119.53	105.20
32	1a	657	G	N3-C4-N9	-6.51	122.09	126.00
32	1a	756	C	C5-C6-N1	-6.51	117.75	121.00
1	2A	1115	G	N1-C6-O6	-6.51	115.99	119.90
1	1A	713	G	N9-C4-C5	-6.51	102.80	105.40
1	2A	659	C	O5'-P-OP2	-6.51	99.84	105.70
1	2A	1786	A	O4'-C1'-N9	6.51	113.41	108.20
1	1A	2557	G	O5'-P-OP1	6.51	118.51	110.70
1	1A	339	U	N3-C4-O4	-6.51	114.85	119.40
1	1A	607	U	O5'-P-OP2	-6.51	99.84	105.70
1	2A	2526	G	N1-C6-O6	6.51	123.80	119.90
1	1A	1303	G	C5-C6-O6	6.50	132.50	128.60
32	1a	35	G	C8-N9-C4	-6.50	103.80	106.40
32	2a	1418	A	O5'-P-OP2	6.50	118.51	110.70
1	1A	2628	C	C5-C6-N1	-6.50	117.75	121.00
1	2A	2540	C	O5'-P-OP2	-6.50	99.85	105.70
2	2B	117	G	N1-C6-O6	6.50	123.80	119.90
32	2a	472	A	C8-N9-C4	-6.50	103.20	105.80
1	1A	1430	C	C6-N1-C2	-6.50	117.70	120.30
1	2A	2286	A	O4'-C1'-N9	-6.50	103.00	108.20
1	1A	1455	G	C6-C5-N7	-6.50	126.50	130.40
1	1A	2620	C	N1-C2-O2	6.50	122.80	118.90
32	1a	225	C	C6-N1-C2	6.50	122.90	120.30
1	2A	2182	G	N9-C4-C5	6.50	108.00	105.40
1	2A	2238	G	OP1-P-OP2	6.50	129.35	119.60
1	1A	141	A	C8-N9-C4	6.50	108.40	105.80
1	1A	614	U	N1-C2-N3	6.50	118.80	114.90
1	1A	1427	A	C4-C5-N7	-6.50	107.45	110.70
1	1A	1817	G	N7-C8-N9	6.50	116.35	113.10
1	1A	2507	C	O5'-P-OP1	-6.50	99.85	105.70
32	1a	1016	A	N1-C6-N6	6.50	122.50	118.60
1	2A	1567	A	C8-N9-C4	6.50	108.40	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1978	A	N1-C2-N3	6.50	132.55	129.30
32	2a	903	G	N1-C6-O6	6.50	123.80	119.90
1	1A	2036	C	C2-N3-C4	-6.50	116.65	119.90
1	1A	2037	G	O5'-P-OP2	-6.50	99.86	105.70
1	2A	589	C	C6-N1-C2	-6.50	117.70	120.30
1	2A	1678	G	N7-C8-N9	6.50	116.35	113.10
1	1A	125	G	O4'-C1'-N9	-6.49	103.00	108.20
1	1A	768	G	C5-C6-O6	-6.49	124.70	128.60
1	1A	2314	C	C2-N1-C1'	-6.49	111.66	118.80
1	1A	2578	G	C6-C5-N7	6.49	134.30	130.40
1	1A	2590	A	N7-C8-N9	6.49	117.05	113.80
32	2a	908	A	C8-N9-C4	6.49	108.40	105.80
1	1A	271(V)	G	N1-C6-O6	6.49	123.80	119.90
1	1A	1295	C	C5-C6-N1	-6.49	117.75	121.00
1	1A	1699	G	N1-C6-O6	-6.49	116.00	119.90
1	2A	34	C	C6-N1-C2	-6.49	117.70	120.30
1	2A	98	G	C2-N3-C4	-6.49	108.65	111.90
1	2A	1891	G	N3-C2-N2	-6.49	115.36	119.90
1	1A	2369	A	N9-C4-C5	6.49	108.39	105.80
1	1A	1008	C	C2-N3-C4	6.49	123.14	119.90
1	1A	1670	C	N3-C4-N4	-6.49	113.46	118.00
1	1A	2047	U	OP2-P-O3'	6.49	119.47	105.20
1	2A	59	U	N3-C4-C5	-6.49	110.71	114.60
1	1A	1219	G	C8-N9-C4	6.48	108.99	106.40
1	1A	785	G	N1-C2-N2	6.48	122.03	116.20
32	1a	1486	G	N1-C6-O6	6.48	123.79	119.90
4	1E	102	VAL	CB-CA-C	-6.48	99.09	111.40
1	2A	398	G	C8-N9-C4	6.48	108.99	106.40
1	2A	2105	C	C6-N1-C2	-6.48	117.71	120.30
4	2E	136	ARG	NE-CZ-NH1	-6.48	117.06	120.30
1	2A	2685	G	C5-C6-O6	6.48	132.49	128.60
1	1A	382	G	C8-N9-C4	6.48	108.99	106.40
1	1A	2528	U	C6-N1-C2	-6.48	117.11	121.00
1	2A	242	G	N7-C8-N9	-6.48	109.86	113.10
32	2a	1524	C	C6-N1-C2	6.48	122.89	120.30
2	1B	98	G	C4-C5-N7	6.48	113.39	110.80
1	1A	335	C	C6-N1-C2	-6.47	117.71	120.30
32	1a	1287	A	C8-N9-C4	-6.47	103.21	105.80
1	2A	772	C	C6-N1-C2	-6.47	117.71	120.30
1	2A	1032	A	C5-N7-C8	-6.47	100.66	103.90
1	2A	1635	G	N1-C6-O6	6.47	123.78	119.90
1	2A	2733	A	N7-C8-N9	6.47	117.04	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	470	A	N1-C2-N3	6.47	132.54	129.30
1	1A	1284	A	C6-C5-N7	-6.47	127.77	132.30
1	1A	2419	U	N3-C4-O4	-6.47	114.87	119.40
1	1A	2628	C	N1-C2-O2	6.47	122.78	118.90
1	2A	578	A	C8-N9-C4	6.47	108.39	105.80
1	2A	1270	C	N3-C4-N4	-6.47	113.47	118.00
1	2A	2784	C	N3-C2-O2	-6.47	117.37	121.90
32	2a	721	G	C5-C6-N1	-6.47	108.26	111.50
1	1A	1791	A	OP1-P-OP2	-6.47	109.89	119.60
1	1A	2038	G	C2-N3-C4	6.47	115.14	111.90
1	1A	1801	G	C8-N9-C4	-6.47	103.81	106.40
32	1a	380	G	C5-C6-O6	6.47	132.48	128.60
32	2a	266	G	P-O3'-C3'	6.47	127.46	119.70
32	2a	430	A	N1-C6-N6	6.47	122.48	118.60
32	2a	826	C	C6-N1-C2	6.47	122.89	120.30
1	1A	1309	G	C2-N3-C4	-6.47	108.67	111.90
1	2A	2718	G	C8-N9-C4	-6.47	103.81	106.40
32	2a	698	G	N1-C6-O6	6.47	123.78	119.90
1	1A	261	G	N3-C2-N2	-6.47	115.37	119.90
1	1A	2027	G	N1-C6-O6	-6.47	116.02	119.90
1	1A	2328	A	C4-C5-C6	6.47	120.23	117.00
4	1E	16	ARG	NE-CZ-NH1	-6.47	117.07	120.30
1	1A	1686	C	C6-N1-C2	-6.46	117.71	120.30
1	1A	2614	A	N7-C8-N9	-6.46	110.57	113.80
2	1B	87	G	C8-N9-C4	6.46	108.99	106.40
1	2A	53	A	N1-C2-N3	6.46	132.53	129.30
1	2A	2423	U	C5-C6-N1	-6.46	119.47	122.70
30	18	62	LEU	CB-CG-CD1	-6.46	100.01	111.00
32	2a	789	U	C5-C6-N1	-6.46	119.47	122.70
1	1A	2445	G	N1-C6-O6	-6.46	116.02	119.90
1	1A	2711	A	C2-N3-C4	-6.46	107.37	110.60
32	1a	831	U	C6-N1-C2	-6.46	117.12	121.00
1	2A	2356	C	N1-C2-O2	-6.46	115.02	118.90
1	1A	513	A	C8-N9-C1'	-6.46	116.07	127.70
1	2A	329	G	C6-N1-C2	-6.46	121.22	125.10
1	1A	64	A	C6-N1-C2	-6.46	114.72	118.60
1	1A	2483	C	N3-C4-N4	6.46	122.52	118.00
32	1a	1018	C	C6-N1-C2	-6.46	117.72	120.30
1	2A	782	A	N1-C2-N3	6.46	132.53	129.30
1	1A	815	C	N1-C2-O2	-6.46	115.03	118.90
1	1A	1187	G	C5-N7-C8	-6.46	101.07	104.30
1	1A	1838	C	N3-C2-O2	-6.46	117.38	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	535	C	N1-C2-O2	6.46	122.77	118.90
1	2A	2018	G	N1-C2-N3	-6.46	120.03	123.90
32	2a	34	C	C6-N1-C2	6.46	122.88	120.30
32	1a	578	C	OP2-P-O3'	6.46	119.40	105.20
1	1A	226	G	C8-N9-C4	-6.45	103.82	106.40
1	1A	1203	G	N1-C6-O6	6.45	123.77	119.90
1	1A	1331	A	OP1-P-O3'	-6.45	91.00	105.20
1	1A	2013	A	N1-C6-N6	-6.45	114.73	118.60
1	1A	1192	G	C2-N3-C4	-6.45	108.67	111.90
1	1A	1805	U	N1-C2-N3	6.45	118.77	114.90
1	1A	2406	U	O4'-C1'-N1	-6.45	103.04	108.20
1	1A	2639	A	C4-C5-N7	6.45	113.92	110.70
32	1a	1493	A	C8-N9-C4	-6.45	103.22	105.80
1	2A	2010	G	O5'-P-OP1	-6.45	99.89	105.70
1	2A	2468	G	N3-C2-N2	-6.45	115.38	119.90
1	1A	306	U	N3-C4-C5	-6.45	110.73	114.60
1	1A	1975	G	N9-C4-C5	-6.45	102.82	105.40
32	1a	1328	C	C6-N1-C2	6.45	122.88	120.30
32	1a	1403	C	C5-C4-N4	6.45	124.71	120.20
1	2A	2018	G	O5'-P-OP1	6.45	118.44	110.70
32	2a	1230	C	N1-C2-O2	6.45	122.77	118.90
1	1A	154(A)	C	C6-N1-C2	6.45	122.88	120.30
1	1A	488	G	N1-C2-N3	6.45	127.77	123.90
1	2A	1606	G	C6-C5-N7	-6.45	126.53	130.40
1	1A	206	U	N1-C2-O2	-6.45	118.29	122.80
1	1A	366	C	N3-C2-O2	6.45	126.41	121.90
1	1A	122	G	C5-C6-O6	-6.44	124.73	128.60
1	1A	949	C	N3-C4-C5	-6.44	119.32	121.90
1	2A	540	C	N1-C2-O2	6.44	122.77	118.90
1	2A	798	G	C4-C5-N7	-6.44	108.22	110.80
1	2A	993	G	C8-N9-C1'	6.44	135.38	127.00
1	1A	1573	G	C8-N9-C4	6.44	108.98	106.40
1	1A	1627	G	O5'-P-OP2	-6.44	99.90	105.70
1	1A	582	G	C5-N7-C8	-6.44	101.08	104.30
1	1A	1241	A	N1-C6-N6	6.44	122.47	118.60
1	2A	251	A	N1-C2-N3	6.44	132.52	129.30
1	2A	906	G	N1-C6-O6	-6.44	116.04	119.90
1	2A	749	C	N3-C4-N4	6.44	122.51	118.00
1	1A	1231	G	C5-C6-O6	6.44	132.46	128.60
1	1A	967	C	C5-C6-N1	-6.43	117.78	121.00
1	1A	1756	G	N9-C4-C5	6.43	107.97	105.40
1	1A	1774	C	C5-C4-N4	-6.43	115.70	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	911	A	C4-C5-N7	6.43	113.92	110.70
1	1A	1231	G	C5-C6-N1	-6.43	108.28	111.50
32	1a	857	C	N3-C4-C5	-6.43	119.33	121.90
1	2A	365	C	N3-C4-C5	-6.43	119.33	121.90
1	2A	450	G	N9-C4-C5	6.43	107.97	105.40
1	1A	975(A)	G	N3-C4-N9	-6.43	122.14	126.00
32	1a	298	A	N1-C2-N3	6.43	132.51	129.30
32	1a	912	C	N1-C2-O2	-6.43	115.04	118.90
1	1A	125	G	N9-C4-C5	-6.43	102.83	105.40
1	1A	1831	G	C8-N9-C4	-6.43	103.83	106.40
1	1A	2335	A	N1-C6-N6	-6.43	114.74	118.60
1	1A	2388	A	O4'-C1'-N9	6.43	113.34	108.20
2	1B	63	G	N7-C8-N9	-6.43	109.89	113.10
1	2A	1222	C	C6-N1-C2	6.43	122.87	120.30
32	2a	588	G	O5'-P-OP2	-6.43	99.92	105.70
32	2a	1063	C	C6-N1-C2	-6.43	117.73	120.30
1	1A	2233	U	N1-C2-N3	6.43	118.76	114.90
1	1A	2540	C	C6-N1-C2	6.43	122.87	120.30
1	2A	1959	G	N1-C6-O6	-6.43	116.05	119.90
1	1A	306	U	C4-C5-C6	6.42	123.55	119.70
1	1A	2578	G	N9-C4-C5	6.42	107.97	105.40
1	1A	574	C	N3-C2-O2	-6.42	117.41	121.90
1	1A	797	C	OP1-P-OP2	-6.42	109.97	119.60
1	1A	2690	C	N1-C2-O2	-6.42	115.05	118.90
1	1A	2687	U	N3-C4-C5	-6.42	110.75	114.60
1	2A	961	C	OP1-P-OP2	6.42	129.23	119.60
32	2a	791	G	C6-C5-N7	-6.42	126.55	130.40
1	1A	197	A	O5'-P-OP1	-6.42	99.92	105.70
1	2A	1858	G	O4'-C1'-N9	6.42	113.33	108.20
32	2a	357	G	C5-C6-N1	-6.42	108.29	111.50
1	1A	668	G	N3-C4-C5	-6.42	125.39	128.60
1	1A	1272	A	C6-N1-C2	-6.42	114.75	118.60
1	1A	1681	G	N1-C6-O6	-6.42	116.05	119.90
1	1A	1757	U	C6-N1-C2	6.42	124.85	121.00
1	2A	2833	G	C8-N9-C4	6.42	108.97	106.40
32	1a	882	C	C6-N1-C2	-6.42	117.73	120.30
1	2A	909	A	C8-N9-C4	-6.42	103.23	105.80
1	2A	1930	G	C5-N7-C8	6.42	107.51	104.30
1	1A	399	G	O5'-P-OP1	6.41	118.40	110.70
3	1D	215	LEU	CB-CG-CD2	-6.41	100.10	111.00
32	1a	1397	C	N1-C2-O2	6.41	122.75	118.90
1	2A	1370	C	O5'-P-OP1	-6.41	99.93	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2092	U	OP1-P-OP2	6.41	129.22	119.60
1	2A	219	G	N1-C2-N3	6.41	127.75	123.90
1	1A	981	A	OP2-P-O3'	6.41	119.30	105.20
32	1a	266	G	C8-N9-C4	-6.41	103.84	106.40
1	2A	2658	C	C5-C6-N1	-6.41	117.80	121.00
32	2a	866	C	C6-N1-C2	-6.41	117.74	120.30
1	1A	139(A)	G	C2-N3-C4	-6.41	108.70	111.90
1	1A	244	A	C6-C5-N7	-6.41	127.82	132.30
1	1A	504	U	OP2-P-O3'	6.41	119.29	105.20
1	1A	636	G	N3-C2-N2	-6.41	115.42	119.90
1	1A	1622	G	C6-C5-N7	6.40	134.24	130.40
1	1A	1839	G	O4'-C1'-N9	-6.40	103.08	108.20
1	2A	2768	C	C6-N1-C2	-6.40	117.74	120.30
1	1A	127	A	C8-N9-C4	6.40	108.36	105.80
1	1A	2624	G	O5'-P-OP1	6.40	118.38	110.70
32	1a	1505	G	N3-C4-N9	-6.40	122.16	126.00
1	1A	858	U	O5'-P-OP2	-6.40	99.94	105.70
1	1A	2197	U	N3-C2-O2	6.40	126.68	122.20
1	1A	2488	A	C5-C6-N1	6.40	120.90	117.70
1	1A	2540	C	N3-C4-N4	-6.40	113.52	118.00
1	1A	2687	U	N3-C2-O2	6.40	126.68	122.20
1	2A	768	G	C5-C6-O6	-6.40	124.76	128.60
1	2A	1661	G	N1-C6-O6	6.40	123.74	119.90
21	2Z	41	LEU	CA-CB-CG	-6.40	100.58	115.30
32	2a	1497	G	O5'-P-OP2	-6.40	99.94	105.70
1	1A	83	G	N3-C4-N9	6.40	129.84	126.00
32	1a	913	A	P-O3'-C3'	6.40	127.38	119.70
1	2A	1032	A	N3-C4-C5	6.40	131.28	126.80
1	1A	126	A	C5-C6-N1	-6.40	114.50	117.70
2	1B	72	G	O5'-P-OP2	-6.40	99.94	105.70
1	2A	936	C	N3-C4-C5	6.40	124.46	121.90
1	2A	2435	A	C2-N3-C4	-6.40	107.40	110.60
1	1A	917	A	C8-N9-C4	6.40	108.36	105.80
32	1a	982	U	C5-C6-N1	-6.39	119.50	122.70
1	2A	704	G	C5-C6-O6	6.39	132.44	128.60
1	2A	2353	G	OP1-P-OP2	6.39	129.19	119.60
1	1A	15	G	N3-C2-N2	-6.39	115.42	119.90
1	1A	2537	U	C5-C4-O4	6.39	129.74	125.90
1	2A	1769	G	N1-C6-O6	6.39	123.74	119.90
1	2A	2231	C	N3-C4-C5	-6.39	119.34	121.90
1	2A	2709	G	N3-C4-C5	6.39	131.80	128.60
1	1A	193	U	N3-C4-O4	6.39	123.87	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1510	G	N1-C6-O6	6.39	123.73	119.90
1	1A	2685	G	N9-C4-C5	6.39	107.96	105.40
32	1a	1447	A	O4'-C1'-N9	6.39	113.31	108.20
1	1A	1658	C	C4-C5-C6	6.39	120.59	117.40
1	1A	1680	U	C5-C4-O4	6.39	129.73	125.90
1	2A	1551	C	C6-N1-C2	-6.39	117.74	120.30
1	2A	1826	G	C5-N7-C8	6.39	107.50	104.30
1	1A	1958	C	O5'-P-OP1	6.39	118.36	110.70
32	2a	871	U	N1-C2-O2	6.39	127.27	122.80
1	1A	218	A	N1-C6-N6	-6.39	114.77	118.60
1	1A	1525	G	OP1-P-OP2	6.39	129.18	119.60
1	1A	1677	A	O5'-P-OP2	-6.39	99.95	105.70
1	1A	2371	G	N1-C6-O6	-6.39	116.07	119.90
1	2A	1365	A	C5-C6-N6	6.39	128.81	123.70
1	2A	1776	G	C6-C5-N7	-6.39	126.57	130.40
1	1A	456	C	C6-N1-C2	6.38	122.85	120.30
32	1a	1067	A	C8-N9-C4	-6.38	103.25	105.80
32	1a	854	G	O5'-P-OP1	-6.38	99.95	105.70
1	2A	2679	A	C8-N9-C4	6.38	108.35	105.80
1	1A	298	G	N7-C8-N9	-6.38	109.91	113.10
1	1A	698	C	C4-C5-C6	6.38	120.59	117.40
1	1A	2525	G	O5'-P-OP2	-6.38	99.96	105.70
32	1a	163	C	N1-C2-O2	6.38	122.73	118.90
1	2A	2378	A	N9-C4-C5	-6.38	103.25	105.80
1	1A	226	G	N3-C4-C5	-6.38	125.41	128.60
1	1A	1648	C	OP1-P-OP2	-6.38	110.03	119.60
1	1A	2355	C	C5-C6-N1	-6.38	117.81	121.00
32	2a	948	C	O5'-P-OP2	-6.38	99.96	105.70
1	1A	2582	G	O5'-P-OP2	6.38	118.35	110.70
1	2A	2764	A	C2-N3-C4	-6.38	107.41	110.60
1	1A	189	G	N1-C6-O6	6.38	123.72	119.90
1	2A	2102	U	N1-C2-O2	6.38	127.26	122.80
32	2a	343	U	O4'-C1'-N1	6.38	113.30	108.20
1	1A	446	G	N1-C6-O6	6.38	123.72	119.90
1	1A	622	G	C2-N3-C4	-6.38	108.71	111.90
1	1A	2020	A	N1-C2-N3	6.38	132.49	129.30
1	2A	2048	G	C8-N9-C4	-6.38	103.85	106.40
32	2a	993	G	N3-C4-C5	-6.38	125.41	128.60
1	1A	113	G	N1-C6-O6	6.37	123.72	119.90
1	1A	1259	G	N3-C2-N2	-6.37	115.44	119.90
1	1A	1666	G	C5-C6-O6	6.37	132.42	128.60
2	1B	87	G	N9-C4-C5	-6.37	102.85	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	504	U	C2-N1-C1'	6.37	125.35	117.70
1	2A	1239	G	N1-C6-O6	6.37	123.72	119.90
1	1A	1189	A	C8-N9-C4	6.37	108.35	105.80
1	1A	2407	G	C4-N9-C1'	6.37	134.78	126.50
25	13	31	LEU	CB-CG-CD1	-6.37	100.17	111.00
1	2A	721	C	C5-C6-N1	-6.37	117.81	121.00
1	2A	1780	A	C2-N3-C4	-6.37	107.42	110.60
1	2A	1835	G	C2-N3-C4	-6.37	108.71	111.90
1	2A	2585	U	C5-C4-O4	-6.37	122.08	125.90
1	2A	2683	C	N3-C4-C5	-6.37	119.35	121.90
1	2A	2689	U	N3-C2-O2	-6.37	117.74	122.20
1	1A	124	G	C2-N3-C4	-6.37	108.72	111.90
1	1A	527	C	C6-N1-C2	6.37	122.85	120.30
1	2A	228	A	C5-C6-N1	6.37	120.89	117.70
1	2A	645	C	N3-C2-O2	-6.37	117.44	121.90
1	1A	772	C	OP2-P-O3'	6.37	119.21	105.20
1	1A	1047	G	N3-C2-N2	6.37	124.36	119.90
1	1A	1428	C	C2-N1-C1'	-6.37	111.79	118.80
1	2A	827	U	OP1-P-OP2	-6.37	110.05	119.60
1	2A	1791	A	C8-N9-C4	-6.37	103.25	105.80
1	1A	777	A	N1-C2-N3	6.37	132.48	129.30
1	1A	1800	C	C4-C5-C6	6.37	120.58	117.40
1	1A	1976	U	C6-N1-C2	-6.37	117.18	121.00
32	1a	948	C	C6-N1-C2	6.37	122.85	120.30
1	2A	1159	U	O5'-P-OP2	-6.37	99.97	105.70
1	2A	1426	G	C8-N9-C4	6.37	108.95	106.40
1	1A	702	G	N9-C4-C5	-6.36	102.85	105.40
1	1A	733	G	C8-N9-C1'	-6.36	118.73	127.00
32	1a	1516	G	C4-N9-C1'	-6.36	118.23	126.50
1	2A	932	G	C4-N9-C1'	-6.36	118.23	126.50
32	2a	92	C	N1-C2-O2	6.36	122.72	118.90
32	2a	896	C	C5-C6-N1	-6.36	117.82	121.00
1	1A	1286	A	C5-C6-N6	6.36	128.79	123.70
1	1A	1325	G	N9-C4-C5	6.36	107.94	105.40
1	2A	2643	G	O5'-P-OP1	-6.36	99.97	105.70
1	2A	451	C	C5-C6-N1	-6.36	117.82	121.00
1	2A	1265	A	C2-N3-C4	-6.36	107.42	110.60
1	1A	1456	G	C5-C6-O6	-6.36	124.78	128.60
32	1a	570	G	N1-C6-O6	6.36	123.72	119.90
32	1a	1506	U	N3-C4-O4	6.36	123.85	119.40
1	1A	504	U	C2-N1-C1'	6.36	125.33	117.70
1	1A	789	A	C2-N3-C4	-6.36	107.42	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1784	A	N7-C8-N9	-6.36	110.62	113.80
1	2A	147	U	C2-N1-C1'	-6.36	110.07	117.70
1	1A	601	C	N3-C2-O2	-6.36	117.45	121.90
32	2a	266	G	O4'-C1'-N9	-6.35	103.12	108.20
1	1A	1091	G	N3-C4-C5	-6.35	125.42	128.60
1	1A	1416	G	O4'-C1'-N9	6.35	113.28	108.20
1	2A	171	G	N1-C6-O6	-6.35	116.09	119.90
1	2A	2497	A	C8-N9-C4	6.35	108.34	105.80
32	2a	493	G	O5'-P-OP1	-6.35	99.98	105.70
1	1A	1241	A	N9-C4-C5	-6.35	103.26	105.80
1	1A	2333	A	OP1-P-O3'	6.35	119.17	105.20
1	2A	693	C	N1-C2-O2	-6.35	115.09	118.90
1	1A	205	G	N3-C4-N9	6.35	129.81	126.00
1	1A	822	U	N1-C2-O2	-6.35	118.36	122.80
1	1A	1631	C	N1-C2-O2	-6.35	115.09	118.90
1	1A	1666	G	C4-C5-N7	-6.35	108.26	110.80
32	1a	783	C	O5'-P-OP2	-6.35	99.98	105.70
1	2A	1759	A	N1-C2-N3	6.35	132.47	129.30
8	2I	38	LEU	CA-CB-CG	6.35	129.91	115.30
32	2a	41	G	N3-C2-N2	-6.35	115.45	119.90
1	1A	784	A	OP2-P-O3'	6.35	119.17	105.20
1	1A	2433	A	N7-C8-N9	6.35	116.97	113.80
32	2a	1397	C	C5-C6-N1	6.35	124.17	121.00
1	1A	1404	C	C5-C4-N4	6.35	124.64	120.20
1	1A	1520	G	N9-C4-C5	6.35	107.94	105.40
1	2A	1721	G	N3-C2-N2	6.35	124.34	119.90
1	2A	2362	G	N1-C6-O6	-6.35	116.09	119.90
1	2A	2572	A	C4-C5-N7	-6.35	107.53	110.70
1	1A	1246	A	C2-N3-C4	-6.34	107.43	110.60
1	1A	2056	G	C4-C5-N7	6.34	113.34	110.80
1	2A	675	A	C2-N3-C4	-6.34	107.43	110.60
1	2A	761	A	N1-C2-N3	6.34	132.47	129.30
1	2A	1225	G	C4-C5-N7	-6.34	108.26	110.80
1	2A	1405	U	O5'-P-OP2	-6.34	99.99	105.70
1	2A	2700	C	C6-N1-C2	6.34	122.84	120.30
1	1A	2227	A	OP2-P-O3'	6.34	119.16	105.20
32	1a	618	C	C2-N3-C4	6.34	123.07	119.90
1	2A	1951	U	N1-C2-O2	6.34	127.24	122.80
32	2a	70	G	N1-C6-O6	6.34	123.71	119.90
1	1A	1436	G	N1-C6-O6	6.34	123.70	119.90
1	1A	1955	U	N3-C2-O2	6.34	126.64	122.20
1	1A	2746	U	N3-C4-O4	-6.34	114.96	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1899	G	C6-N1-C2	-6.34	121.30	125.10
1	2A	2568	C	C6-N1-C2	6.34	122.84	120.30
1	1A	1218	C	N1-C2-N3	-6.34	114.76	119.20
1	1A	1888	G	C5-N7-C8	-6.34	101.13	104.30
1	1A	2027	G	C4-C5-N7	-6.34	108.27	110.80
1	1A	2043	C	N3-C4-N4	6.34	122.44	118.00
1	1A	2278	A	C2-N3-C4	-6.34	107.43	110.60
1	1A	2568	C	C6-N1-C2	6.34	122.84	120.30
1	2A	1311	G	N3-C4-N9	6.34	129.80	126.00
1	1A	800	A	O5'-P-OP1	-6.34	100.00	105.70
1	1A	1204	A	C2-N3-C4	-6.34	107.43	110.60
1	2A	1381	G	OP2-P-O3'	6.34	119.14	105.20
1	2A	2323	G	N3-C4-C5	6.34	131.77	128.60
1	1A	472	A	OP2-P-O3'	6.34	119.14	105.20
1	1A	1975	G	O5'-P-OP2	-6.34	100.00	105.70
24	12	59	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	1A	2647	U	C4-C5-C6	6.33	123.50	119.70
1	2A	187	G	N1-C6-O6	6.33	123.70	119.90
1	1A	660	G	N1-C6-O6	6.33	123.70	119.90
2	1B	31	C	O5'-P-OP2	-6.33	100.00	105.70
1	2A	1618	A	N9-C4-C5	6.33	108.33	105.80
1	2A	2332	U	N3-C2-O2	-6.33	117.77	122.20
1	1A	772	C	C2-N1-C1'	6.33	125.76	118.80
2	1B	79	C	C5-C6-N1	-6.33	117.83	121.00
1	2A	37	C	C6-N1-C2	6.33	122.83	120.30
1	2A	710	G	N1-C6-O6	6.33	123.70	119.90
1	2A	1423	G	C2-N3-C4	-6.33	108.73	111.90
1	2A	1600	C	N1-C2-O2	-6.33	115.10	118.90
32	2a	1278	U	N3-C2-O2	-6.33	117.77	122.20
1	1A	1121	C	C6-N1-C2	-6.33	117.77	120.30
32	1a	1319	A	C5-C6-N6	6.33	128.76	123.70
1	2A	2246	G	C2-N3-C4	-6.33	108.74	111.90
1	1A	2005	A	C5-C6-N1	6.33	120.86	117.70
1	1A	1805	U	N1-C2-O2	-6.33	118.37	122.80
1	1A	2206	G	C4-N9-C1'	-6.33	118.28	126.50
1	1A	2518	A	N7-C8-N9	6.33	116.96	113.80
1	1A	2858	C	OP1-P-OP2	6.32	129.09	119.60
4	1E	82	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	2A	527	C	C5-C6-N1	-6.32	117.84	121.00
1	2A	2652	C	O5'-P-OP2	-6.32	100.01	105.70
1	1A	2639	A	N9-C4-C5	-6.32	103.27	105.80
32	2a	1495	U	C6-N1-C2	-6.32	117.21	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	401	A	C2-N3-C4	-6.32	107.44	110.60
1	1A	1254	A	C6-N1-C2	-6.32	114.81	118.60
1	1A	1455	G	N9-C4-C5	-6.32	102.87	105.40
1	1A	2662	A	C6-C5-N7	-6.32	127.88	132.30
1	2A	194	G	N1-C6-O6	6.32	123.69	119.90
1	2A	2220	G	N3-C2-N2	-6.32	115.48	119.90
1	1A	681	G	OP1-P-OP2	6.32	129.08	119.60
1	1A	1373	A	C8-N9-C4	6.32	108.33	105.80
1	2A	1175	U	P-O3'-C3'	6.32	127.28	119.70
1	2A	2230	G	OP1-P-OP2	6.32	129.08	119.60
32	2a	404	U	C6-N1-C1'	-6.32	112.35	121.20
1	1A	572	A	N9-C4-C5	6.32	108.33	105.80
1	1A	788	A	OP2-P-O3'	6.32	119.10	105.20
1	1A	928	G	N9-C4-C5	-6.32	102.87	105.40
1	1A	954	G	N1-C2-N3	6.32	127.69	123.90
32	1a	818	G	N1-C6-O6	-6.32	116.11	119.90
1	2A	272	G	C6-C5-N7	-6.32	126.61	130.40
1	2A	620	G	C8-N9-C4	-6.32	103.87	106.40
1	2A	1686	C	C5-C6-N1	-6.32	117.84	121.00
1	1A	1944	U	C5-C6-N1	-6.32	119.54	122.70
1	1A	2331	G	N9-C4-C5	-6.32	102.87	105.40
1	1A	2509	G	N3-C2-N2	6.32	124.32	119.90
2	1B	89	G	C6-C5-N7	-6.32	126.61	130.40
32	1a	1467	G	C4-C5-N7	-6.32	108.27	110.80
1	2A	2038	G	N7-C8-N9	-6.32	109.94	113.10
1	2A	2468	G	N3-C4-N9	-6.32	122.21	126.00
2	2B	116	G	C8-N9-C4	6.32	108.93	106.40
1	1A	779	U	OP1-P-OP2	-6.31	110.13	119.60
1	2A	1661	G	C4-C5-N7	6.31	113.33	110.80
32	2a	163	C	N3-C4-C5	-6.31	119.38	121.90
32	2a	1290	G	C8-N9-C4	-6.31	103.88	106.40
1	1A	1973	G	O5'-P-OP1	-6.31	100.02	105.70
1	2A	755	C	OP2-P-O3'	6.31	119.08	105.20
32	2a	687	A	O5'-P-OP1	-6.31	100.02	105.70
1	1A	271	A	C5-C6-N6	-6.31	118.65	123.70
1	1A	947	G	N1-C2-N2	6.31	121.88	116.20
1	1A	1681	G	N3-C2-N2	6.31	124.31	119.90
32	2a	898	G	N9-C4-C5	-6.31	102.88	105.40
32	1a	326	G	C4-C5-N7	-6.31	108.28	110.80
1	1A	69	C	OP2-P-O3'	6.30	119.07	105.20
1	1A	2397	G	C5-N7-C8	-6.30	101.15	104.30
1	1A	2711	A	C8-N9-C4	6.30	108.32	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2344	U	C5-C6-N1	-6.30	119.55	122.70
1	1A	2825	C	C5-C4-N4	-6.30	115.79	120.20
1	2A	1253	A	C5-N7-C8	6.30	107.05	103.90
1	1A	620	G	C6-C5-N7	-6.30	126.62	130.40
1	1A	2538	C	C6-N1-C2	6.30	122.82	120.30
32	1a	700	G	OP1-P-OP2	6.30	129.05	119.60
1	2A	94(A)	G	N3-C4-C5	-6.30	125.45	128.60
1	2A	2427	C	N1-C2-O2	-6.30	115.12	118.90
1	1A	154(A)	C	N3-C4-C5	6.30	124.42	121.90
1	1A	1008	C	C2-N1-C1'	6.30	125.73	118.80
1	1A	1307	A	C5-N7-C8	6.30	107.05	103.90
1	1A	1592	C	C6-N1-C2	6.30	122.82	120.30
1	1A	2813	A	C2-N3-C4	-6.30	107.45	110.60
32	1a	1521	G	C4-C5-N7	6.30	113.32	110.80
32	2a	1202	G	C5-C6-O6	6.30	132.38	128.60
32	2a	1262	C	N3-C2-O2	-6.30	117.49	121.90
1	1A	214	G	C4-C5-N7	6.30	113.32	110.80
1	1A	1266	G	C4-C5-C6	-6.30	115.02	118.80
1	1A	1378	A	C8-N9-C4	6.30	108.32	105.80
1	1A	754	C	C5-C4-N4	-6.30	115.79	120.20
1	1A	1271	G	C4-C5-N7	-6.30	108.28	110.80
1	2A	1678	G	N1-C6-O6	6.30	123.68	119.90
1	2A	2224	G	C2-N3-C4	-6.30	108.75	111.90
32	2a	115	G	C8-N9-C4	-6.30	103.88	106.40
1	1A	1199	U	O5'-P-OP2	-6.29	100.03	105.70
1	2A	2538	C	C6-N1-C2	6.29	122.82	120.30
1	1A	43	A	N1-C2-N3	6.29	132.45	129.30
1	1A	530	G	O4'-C1'-N9	-6.29	103.17	108.20
32	1a	512	U	C6-N1-C2	-6.29	117.22	121.00
1	2A	1235	G	C8-N9-C4	-6.29	103.88	106.40
32	2a	281	G	O5'-P-OP2	-6.29	100.03	105.70
1	1A	2849	U	N1-C2-O2	-6.29	118.40	122.80
2	1B	72	G	OP1-P-OP2	6.29	129.04	119.60
32	1a	127	G	N3-C4-N9	-6.29	122.22	126.00
32	1a	644	G	O5'-P-OP2	-6.29	100.04	105.70
1	2A	2061	G	N9-C4-C5	-6.29	102.88	105.40
32	2a	299	G	N9-C4-C5	-6.29	102.88	105.40
1	1A	1234	U	C4-C5-C6	6.29	123.47	119.70
1	1A	2506	U	N1-C2-O2	6.29	127.20	122.80
1	2A	1108	U	C2-N1-C1'	6.29	125.25	117.70
1	1A	149	A	C8-N9-C4	6.29	108.31	105.80
1	1A	778	G	O5'-P-OP2	-6.29	100.04	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	892	G	C4-N9-C1'	-6.29	118.32	126.50
1	1A	2343	C	C6-N1-C2	6.29	122.81	120.30
1	1A	2570	G	C8-N9-C4	6.29	108.92	106.40
1	1A	2738	A	N1-C2-N3	6.29	132.44	129.30
1	2A	2499	C	N3-C4-N4	6.29	122.40	118.00
1	1A	1202	C	N3-C4-C5	-6.29	119.39	121.90
1	1A	270	A	C8-N9-C4	6.29	108.31	105.80
1	1A	777	A	N3-C4-C5	-6.29	122.40	126.80
1	1A	1660	C	C5-C4-N4	6.29	124.60	120.20
1	1A	2422	A	O5'-P-OP2	-6.29	100.04	105.70
32	1a	1140	C	C6-N1-C2	-6.29	117.79	120.30
32	1a	1467	G	OP1-P-O3'	6.29	119.03	105.20
32	1a	1505	G	C4-C5-N7	-6.29	108.29	110.80
1	2A	15	G	C4-C5-N7	6.29	113.31	110.80
1	2A	381	G	C2-N3-C4	-6.29	108.76	111.90
1	2A	1222	C	N3-C4-C5	6.29	124.41	121.90
1	2A	1426	G	C5-N7-C8	6.29	107.44	104.30
1	2A	2010	G	C2-N3-C4	-6.29	108.76	111.90
1	1A	1631	C	N3-C2-O2	6.28	126.30	121.90
1	1A	2325	G	OP1-P-OP2	6.28	129.03	119.60
1	1A	2789	C	C6-N1-C1'	6.28	128.34	120.80
1	2A	271(Y)	U	O4'-C1'-N1	6.28	113.23	108.20
1	2A	1031	G	N1-C6-O6	6.28	123.67	119.90
1	2A	1653	G	N9-C4-C5	-6.28	102.89	105.40
1	1A	2431	U	N3-C4-C5	6.28	118.37	114.60
1	1A	1568	G	C6-C5-N7	-6.28	126.63	130.40
1	2A	1328	G	C4-C5-N7	6.28	113.31	110.80
1	1A	806	C	C4-C5-C6	-6.28	114.26	117.40
1	2A	2718	G	N7-C8-N9	6.28	116.24	113.10
32	2a	926	G	C6-C5-N7	-6.28	126.63	130.40
1	1A	951	C	C2-N3-C4	6.28	123.04	119.90
1	1A	1709	U	N1-C2-N3	6.28	118.67	114.90
1	1A	1811	G	OP2-P-O3'	6.28	119.01	105.20
1	1A	2519	U	N3-C2-O2	-6.28	117.81	122.20
32	1a	629	G	C8-N9-C4	-6.28	103.89	106.40
32	1a	1370	G	C6-C5-N7	-6.28	126.63	130.40
1	2A	415	A	C8-N9-C4	6.28	108.31	105.80
1	2A	470	A	N1-C6-N6	6.28	122.37	118.60
18	2W	94	ASP	CB-CG-OD2	6.28	123.95	118.30
1	2A	1780	A	OP1-P-OP2	6.28	129.01	119.60
32	2a	1530	G	N1-C6-O6	6.28	123.67	119.90
1	1A	1054	A	N7-C8-N9	6.27	116.94	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1349	A	O5'-P-OP1	-6.27	100.05	105.70
1	1A	1823	G	C8-N9-C4	6.27	108.91	106.40
1	2A	824	A	N7-C8-N9	-6.27	110.66	113.80
1	1A	667	U	N1-C2-O2	-6.27	118.41	122.80
1	1A	768	G	C6-C5-N7	-6.27	126.64	130.40
1	1A	2038	G	N3-C2-N2	6.27	124.29	119.90
1	2A	330	A	C8-N9-C1'	-6.27	116.41	127.70
1	2A	2645	G	N3-C4-C5	6.27	131.74	128.60
1	1A	442	G	C5-N7-C8	-6.27	101.16	104.30
1	1A	797	C	C6-N1-C2	6.27	122.81	120.30
1	1A	1786	A	C2-N3-C4	-6.27	107.47	110.60
1	1A	2664	G	N1-C6-O6	-6.27	116.14	119.90
32	1a	300	A	N1-C6-N6	6.27	122.36	118.60
1	2A	509	C	N3-C4-C5	-6.27	119.39	121.90
1	1A	2004	G	N3-C4-N9	-6.27	122.24	126.00
2	1B	75	G	N1-C2-N3	6.27	127.66	123.90
1	2A	1240	U	O5'-P-OP1	-6.27	100.06	105.70
1	1A	2224	G	C8-N9-C4	6.27	108.91	106.40
32	1a	1226	C	C6-N1-C2	-6.27	117.79	120.30
1	2A	1036	G	C4-N9-C1'	-6.27	118.35	126.50
1	2A	1620	G	OP1-P-OP2	-6.27	110.20	119.60
1	2A	1818	U	N1-C2-O2	-6.27	118.41	122.80
1	1A	47	C	N3-C2-O2	-6.27	117.51	121.90
1	1A	2508	G	N3-C4-N9	6.27	129.76	126.00
1	2A	1193	G	C4-C5-N7	6.27	113.31	110.80
1	2A	2148	G	O4'-C1'-N9	6.27	113.21	108.20
1	1A	805	G	C5-C6-O6	-6.26	124.84	128.60
1	1A	2003	G	C2-N3-C4	-6.26	108.77	111.90
1	2A	1365	A	N9-C4-C5	6.26	108.31	105.80
1	2A	1500	G	N1-C6-O6	6.26	123.66	119.90
1	2A	1805	U	N3-C2-O2	-6.26	117.81	122.20
1	2A	1964	G	N3-C4-C5	6.26	131.73	128.60
1	2A	2744	G	OP2-P-O3'	6.26	118.98	105.20
32	2a	585	G	C2-N3-C4	6.26	115.03	111.90
1	1A	461	C	N1-C2-O2	-6.26	115.14	118.90
1	2A	749	C	C5-C6-N1	6.26	124.13	121.00
32	2a	481	G	C4-N9-C1'	6.26	134.64	126.50
1	1A	1805	U	C4-C5-C6	6.26	123.46	119.70
1	1A	2001	A	N1-C2-N3	-6.26	126.17	129.30
32	1a	722	A	C4-C5-N7	6.26	113.83	110.70
1	2A	2577	A	N7-C8-N9	6.26	116.93	113.80
32	2a	657	G	N3-C4-C5	6.26	131.73	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1285	A	N1-C6-N6	-6.26	114.84	118.60
1	1A	509	C	C6-N1-C2	6.26	122.80	120.30
1	1A	1976	U	N1-C2-N3	6.26	118.66	114.90
1	1A	2762	G	C8-N9-C4	6.26	108.90	106.40
1	2A	508	G	C5-C6-O6	-6.26	124.84	128.60
1	2A	1426	G	N7-C8-N9	-6.26	109.97	113.10
2	2B	26	A	C8-N9-C4	-6.26	103.30	105.80
32	2a	308	C	C6-N1-C2	6.26	122.80	120.30
1	2A	2720	U	C5-C6-N1	-6.26	119.57	122.70
1	1A	1863	G	N7-C8-N9	-6.26	109.97	113.10
32	1a	421	U	N1-C2-O2	6.26	127.18	122.80
1	2A	171	G	C8-N9-C4	-6.26	103.90	106.40
1	2A	592	G	C4-C5-N7	-6.26	108.30	110.80
1	1A	2227	A	N1-C6-N6	-6.25	114.85	118.60
32	1a	266	G	N7-C8-N9	6.25	116.23	113.10
1	2A	2488	A	N9-C4-C5	-6.25	103.30	105.80
32	2a	306	G	N1-C2-N2	6.25	121.83	116.20
1	1A	2373	G	C8-N9-C4	6.25	108.90	106.40
32	1a	73	G	C8-N9-C1'	6.25	135.13	127.00
1	1A	301	G	O5'-P-OP2	-6.25	100.07	105.70
1	1A	463	G	N1-C2-N3	6.25	127.65	123.90
1	1A	1025	G	N1-C2-N3	6.25	127.65	123.90
1	1A	1122	G	N9-C4-C5	-6.25	102.90	105.40
1	1A	2823	A	C6-C5-N7	-6.25	127.92	132.30
1	2A	1902	C	N1-C2-O2	6.25	122.65	118.90
1	2A	2047	U	N3-C4-C5	6.25	118.35	114.60
1	1A	105	C	O5'-P-OP2	-6.25	100.08	105.70
1	1A	242	G	O4'-C1'-N9	6.25	113.20	108.20
1	1A	978	G	N3-C4-N9	-6.25	122.25	126.00
1	1A	2052	G	C5-N7-C8	-6.25	101.17	104.30
1	1A	517	C	C5-C6-N1	6.25	124.12	121.00
1	1A	2331	G	N3-C4-C5	6.25	131.72	128.60
1	1A	2554	U	N3-C2-O2	6.25	126.57	122.20
1	1A	2678	C	C5-C6-N1	-6.25	117.88	121.00
1	2A	1800	C	C6-N1-C2	-6.25	117.80	120.30
2	2B	115	G	N7-C8-N9	-6.25	109.98	113.10
32	2a	264	U	C6-N1-C1'	-6.25	112.45	121.20
1	1A	750	A	OP2-P-O3'	6.25	118.94	105.20
32	2a	911	U	C5-C4-O4	6.25	129.65	125.90
1	1A	462	C	N3-C2-O2	6.24	126.27	121.90
1	1A	705	A	O4'-C1'-N9	-6.24	103.20	108.20
1	1A	2052	G	N1-C6-O6	6.24	123.65	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1897	G	N1-C6-O6	6.24	123.65	119.90
1	1A	333	G	C8-N9-C1'	-6.24	118.89	127.00
1	1A	1577	C	N3-C2-O2	-6.24	117.53	121.90
1	1A	2369	A	N1-C6-N6	-6.24	114.86	118.60
1	1A	330	A	C6-C5-N7	-6.24	127.93	132.30
1	1A	782	A	O5'-P-OP2	-6.24	100.08	105.70
1	1A	2613	U	OP2-P-O3'	6.24	118.93	105.20
1	2A	807	U	C5-C4-O4	-6.24	122.16	125.90
1	2A	1008	C	N3-C4-N4	-6.24	113.63	118.00
1	2A	2018	G	C5-N7-C8	-6.24	101.18	104.30
32	2a	772	U	C5-C6-N1	-6.24	119.58	122.70
32	2a	1286	A	C8-N9-C4	-6.24	103.30	105.80
32	2a	1465	C	N3-C4-N4	6.24	122.37	118.00
1	1A	1648	C	C6-N1-C2	6.24	122.80	120.30
1	1A	1955	U	N3-C4-C5	6.24	118.34	114.60
1	1A	1956	U	O5'-P-OP1	6.24	118.19	110.70
32	2a	1514	C	N1-C2-O2	-6.24	115.16	118.90
1	2A	1320	C	N3-C2-O2	6.24	126.27	121.90
1	2A	1721	G	N3-C4-N9	6.24	129.74	126.00
1	2A	2041	U	N1-C2-O2	-6.24	118.43	122.80
1	2A	2572	A	N7-C8-N9	-6.24	110.68	113.80
1	1A	702	G	C5-C6-O6	-6.24	124.86	128.60
1	1A	2891	G	N9-C4-C5	-6.24	102.91	105.40
32	1a	1338	G	N1-C6-O6	-6.24	116.16	119.90
1	2A	1619	G	O5'-P-OP2	-6.24	100.09	105.70
1	2A	2549	G	N7-C8-N9	-6.24	109.98	113.10
32	2a	903	G	N9-C4-C5	-6.24	102.91	105.40
1	2A	1351	C	OP1-P-O3'	6.23	118.91	105.20
1	1A	325	G	C5-C6-O6	-6.23	124.86	128.60
1	1A	577	G	OP1-P-OP2	-6.23	110.25	119.60
1	1A	920	G	C6-C5-N7	-6.23	126.66	130.40
1	2A	363	G	N3-C4-N9	-6.23	122.26	126.00
1	2A	2306	C	N1-C2-O2	6.23	122.64	118.90
1	2A	2816	C	N1-C2-O2	-6.23	115.16	118.90
1	1A	198	C	N3-C4-N4	6.23	122.36	118.00
1	1A	402	A	C8-N9-C4	-6.23	103.31	105.80
1	1A	2361	A	N1-C2-N3	6.23	132.41	129.30
32	1a	722	A	N1-C6-N6	6.23	122.34	118.60
1	2A	1976	U	N3-C4-O4	6.23	123.76	119.40
1	2A	2051	A	N1-C6-N6	6.23	122.34	118.60
1	1A	670	A	C5-C6-N6	-6.23	118.72	123.70
1	1A	2066	C	C5-C6-N1	6.23	124.11	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	981	A	C5-C6-N6	-6.23	118.72	123.70
1	1A	1437	C	C6-N1-C2	-6.23	117.81	120.30
1	1A	2235	G	C2-N3-C4	-6.23	108.79	111.90
1	1A	2768	C	N1-C2-O2	-6.23	115.16	118.90
32	1a	805	C	C6-N1-C2	-6.23	117.81	120.30
1	2A	2057	A	N1-C6-N6	-6.23	114.86	118.60
32	2a	980	C	C6-N1-C1'	-6.23	113.33	120.80
1	1A	272(E)	G	C5-C6-O6	-6.23	124.86	128.60
1	1A	1374	G	O5'-P-OP2	6.23	118.17	110.70
1	1A	2087	G	O5'-P-OP2	-6.23	100.10	105.70
1	2A	62	C	C4-C5-C6	6.23	120.51	117.40
1	2A	614	U	N1-C2-N3	6.23	118.64	114.90
1	2A	899	A	C8-N9-C4	-6.23	103.31	105.80
1	1A	1201	C	N3-C4-C5	6.22	124.39	121.90
32	1a	1482	G	N1-C2-N2	-6.22	110.60	116.20
32	2a	1294	G	N3-C4-C5	6.22	131.71	128.60
1	1A	2238	G	OP1-P-OP2	6.22	128.93	119.60
1	2A	527	C	C2-N1-C1'	-6.22	111.95	118.80
1	2A	1385	G	N3-C2-N2	-6.22	115.55	119.90
1	2A	1635	G	O5'-P-OP1	6.22	118.17	110.70
3	2D	215	LEU	CA-CB-CG	-6.22	100.99	115.30
1	1A	944	G	C5-N7-C8	-6.22	101.19	104.30
1	1A	2518	A	C8-N9-C4	-6.22	103.31	105.80
1	1A	1368	G	N3-C4-C5	-6.22	125.49	128.60
1	1A	2433	A	C6-C5-N7	-6.22	127.95	132.30
1	1A	2442	C	N1-C2-O2	-6.22	115.17	118.90
32	1a	578	C	OP1-P-OP2	-6.22	110.27	119.60
32	1a	1525	G	C5-N7-C8	-6.22	101.19	104.30
1	2A	509	C	C6-N1-C2	-6.22	117.81	120.30
1	2A	762	U	N1-C2-O2	6.22	127.15	122.80
1	2A	1866	C	C2-N1-C1'	6.22	125.64	118.80
32	2a	428	G	C4-C5-N7	-6.22	108.31	110.80
1	1A	1614	A	C8-N9-C4	6.22	108.29	105.80
1	1A	2597	G	OP2-P-O3'	6.22	118.88	105.20
1	1A	411	G	N9-C4-C5	6.22	107.89	105.40
1	1A	960	A	C5-C6-N1	6.22	120.81	117.70
1	1A	1438	U	N3-C4-O4	6.22	123.75	119.40
32	1a	26	A	C6-N1-C2	-6.22	114.87	118.60
1	2A	749	C	C2-N1-C1'	6.22	125.64	118.80
1	2A	2871	C	O5'-P-OP2	-6.22	100.11	105.70
1	1A	610	G	N7-C8-N9	-6.21	109.99	113.10
1	1A	1247	A	N1-C2-N3	6.21	132.41	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1495	U	C2-N1-C1'	6.21	125.16	117.70
1	2A	808	G	N1-C6-O6	-6.21	116.17	119.90
1	2A	1184	G	C2-N3-C4	-6.21	108.79	111.90
1	2A	1978	A	C5-C6-N1	-6.21	114.59	117.70
1	2A	2155	G	C2-N3-C4	6.21	115.01	111.90
1	2A	2415	G	C5-C6-N1	-6.21	108.39	111.50
2	2B	55	U	N3-C4-C5	-6.21	110.87	114.60
32	2a	41	G	N1-C6-O6	6.21	123.63	119.90
32	2a	1103	C	C6-N1-C2	-6.21	117.81	120.30
32	2a	1495	U	C5-C6-N1	6.21	125.81	122.70
1	1A	2056	G	N9-C4-C5	-6.21	102.92	105.40
1	2A	2107	C	C6-N1-C2	-6.21	117.81	120.30
1	1A	120	U	C5-C4-O4	6.21	129.63	125.90
1	2A	1314	C	N1-C2-O2	6.21	122.63	118.90
1	2A	1325	G	C8-N9-C4	6.21	108.89	106.40
1	2A	2780	G	O4'-C1'-N9	-6.21	103.23	108.20
32	2a	581	G	C5-C6-O6	-6.21	124.87	128.60
32	1a	1067	A	P-O3'-C3'	6.21	127.15	119.70
1	2A	1567	A	N7-C8-N9	-6.21	110.69	113.80
1	1A	818	G	C4-C5-N7	6.21	113.28	110.80
1	1A	906	G	C8-N9-C1'	6.21	135.07	127.00
1	1A	1099	G	N3-C4-N9	6.21	129.72	126.00
1	1A	1234	U	N3-C4-C5	-6.21	110.88	114.60
1	2A	711	G	N1-C6-O6	6.21	123.63	119.90
1	2A	1826	G	C8-N9-C4	6.21	108.88	106.40
1	2A	1955	U	C2-N1-C1'	-6.21	110.25	117.70
1	1A	190	A	N1-C6-N6	6.21	122.32	118.60
1	1A	637	A	C8-N9-C4	6.21	108.28	105.80
1	2A	2390	U	C2-N1-C1'	6.21	125.15	117.70
1	1A	34	C	O4'-C1'-N1	6.21	113.16	108.20
1	1A	464	U	C5-C4-O4	6.21	129.62	125.90
32	1a	1501	C	C6-N1-C2	6.21	122.78	120.30
1	1A	1382	G	C5-C6-O6	6.20	132.32	128.60
1	1A	1516	C	N1-C2-O2	-6.20	115.18	118.90
1	1A	2334	G	O5'-P-OP1	-6.20	100.12	105.70
32	1a	1035	A	N7-C8-N9	6.20	116.90	113.80
1	2A	2633	G	O5'-P-OP2	-6.20	100.12	105.70
32	2a	719	C	N3-C4-C5	-6.20	119.42	121.90
1	2A	16	G	N1-C6-O6	6.20	123.62	119.90
1	2A	1286	A	N1-C6-N6	-6.20	114.88	118.60
1	1A	1003	G	C2-N3-C4	6.20	115.00	111.90
1	1A	1202	C	N3-C4-N4	6.20	122.34	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1230	C	C5-C6-N1	-6.20	117.90	121.00
1	1A	1622	G	C5-N7-C8	6.20	107.40	104.30
1	1A	2396	G	N3-C4-C5	6.20	131.70	128.60
1	2A	1466	G	C2-N3-C4	6.20	115.00	111.90
1	2A	2076	U	C6-N1-C2	-6.20	117.28	121.00
1	1A	59	U	N3-C4-C5	-6.20	110.88	114.60
1	1A	1332	G	C6-C5-N7	-6.20	126.68	130.40
1	1A	1394	U	C5-C4-O4	6.20	129.62	125.90
1	1A	1774	C	N3-C4-C5	6.20	124.38	121.90
1	1A	2072	G	C6-N1-C2	6.20	128.82	125.10
1	1A	2612	C	O5'-P-OP1	-6.20	100.12	105.70
1	2A	1274	A	N1-C6-N6	6.20	122.32	118.60
1	2A	2224	G	N1-C6-O6	6.20	123.62	119.90
1	2A	2378	A	C8-N9-C1'	-6.20	116.54	127.70
2	1B	51	G	C4-C5-N7	6.20	113.28	110.80
32	2a	1317	C	N1-C2-O2	6.20	122.62	118.90
1	1A	205	G	N3-C2-N2	6.20	124.24	119.90
1	1A	1047	G	C8-N9-C4	-6.20	103.92	106.40
1	1A	2424	C	O5'-P-OP1	-6.20	100.12	105.70
1	1A	2758	A	N1-C6-N6	6.20	122.32	118.60
1	1A	702	G	C8-N9-C4	6.19	108.88	106.40
1	1A	1356	G	O5'-P-OP1	-6.19	100.12	105.70
32	2a	1499	A	N1-C6-N6	6.19	122.32	118.60
1	1A	2049	G	C2-N3-C4	-6.19	108.80	111.90
1	1A	2762	G	C4-N9-C1'	-6.19	118.45	126.50
1	1A	2327	A	C5-C6-N1	6.19	120.80	117.70
11	1P	18	ARG	NE-CZ-NH1	-6.19	117.20	120.30
1	2A	1047	G	N3-C4-C5	-6.19	125.50	128.60
32	2a	1495	U	C2-N3-C4	6.19	130.71	127.00
32	1a	422	C	N1-C2-O2	6.19	122.61	118.90
1	2A	1216	G	C8-N9-C4	-6.19	103.92	106.40
1	1A	632	A	O5'-P-OP2	6.19	118.12	110.70
1	1A	1266	G	C4-N9-C1'	-6.19	118.46	126.50
1	1A	2399	G	C5-C6-O6	6.19	132.31	128.60
1	1A	2498	C	N1-C2-N3	6.19	123.53	119.20
1	1A	2550	G	C8-N9-C4	-6.19	103.92	106.40
1	2A	436	C	N3-C2-O2	-6.19	117.57	121.90
1	2A	2447	G	O5'-P-OP2	6.19	118.13	110.70
1	1A	1009	A	OP1-P-O3'	6.18	118.81	105.20
1	1A	1795	C	C5-C4-N4	-6.18	115.87	120.20
1	1A	2324	C	O5'-P-OP1	6.18	118.12	110.70
2	1B	105	A	N1-C6-N6	6.18	122.31	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	918	A	O5'-P-OP1	-6.18	100.13	105.70
1	2A	391	G	N9-C4-C5	-6.18	102.93	105.40
1	2A	1900	A	C5-C6-N6	-6.18	118.75	123.70
1	2A	2791	C	N3-C4-C5	-6.18	119.43	121.90
1	1A	95	G	N9-C4-C5	6.18	107.87	105.40
1	1A	204	A	C5-N7-C8	-6.18	100.81	103.90
1	1A	227	A	C5-C6-N1	6.18	120.79	117.70
1	1A	246	C	N3-C2-O2	6.18	126.23	121.90
1	1A	272(H)	C	N1-C2-O2	6.18	122.61	118.90
1	1A	2634	G	C5-C6-O6	-6.18	124.89	128.60
32	1a	226	G	N7-C8-N9	-6.18	110.01	113.10
1	1A	2273	A	C5-N7-C8	-6.18	100.81	103.90
1	2A	469	G	C8-N9-C4	6.18	108.87	106.40
1	2A	1818	U	C2-N3-C4	-6.18	123.29	127.00
1	2A	810	U	N3-C4-O4	6.18	123.73	119.40
1	2A	818	G	C5-C6-N1	-6.18	108.41	111.50
1	2A	1064	C	C5-C6-N1	6.18	124.09	121.00
32	2a	500	G	N1-C6-O6	6.18	123.61	119.90
1	1A	2414	G	N1-C6-O6	6.18	123.61	119.90
1	2A	450	G	C4-C5-N7	-6.18	108.33	110.80
1	1A	1041	C	C6-N1-C2	-6.18	117.83	120.30
1	1A	1439	A	O5'-P-OP1	-6.18	100.14	105.70
1	1A	2066	C	N3-C2-O2	6.18	126.22	121.90
1	1A	2249	U	N3-C4-C5	6.18	118.31	114.60
1	2A	764	A	C5-N7-C8	-6.18	100.81	103.90
1	2A	947	G	N3-C4-N9	-6.18	122.29	126.00
1	2A	1834	U	N1-C2-O2	6.18	127.12	122.80
1	2A	2572	A	C5-N7-C8	6.18	106.99	103.90
1	2A	2588	G	C6-N1-C2	6.18	128.81	125.10
1	2A	2821	A	N1-C6-N6	6.18	122.31	118.60
32	2a	1442	G	C8-N9-C1'	-6.18	118.97	127.00
32	1a	15	G	C4-N9-C1'	6.17	134.53	126.50
32	1a	283	C	C2-N1-C1'	6.17	125.59	118.80
1	1A	690	G	N1-C6-O6	6.17	123.60	119.90
32	1a	1435	G	C2-N3-C4	-6.17	108.81	111.90
1	2A	1692	U	N3-C4-C5	-6.17	110.90	114.60
1	2A	2129	C	C6-N1-C2	-6.17	117.83	120.30
32	2a	533	A	N1-C6-N6	6.17	122.30	118.60
32	2a	1037	C	C6-N1-C2	-6.17	117.83	120.30
1	1A	1936	A	C5-N7-C8	-6.17	100.81	103.90
1	1A	2578	G	N1-C6-O6	-6.17	116.20	119.90
1	2A	187	G	C6-C5-N7	-6.17	126.70	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	801	G	N3-C4-C5	6.17	131.69	128.60
32	2a	833	U	C5-C4-O4	6.17	129.60	125.90
32	2a	1442	G	C4-N9-C1'	6.17	134.52	126.50
1	1A	1969	A	C4-C5-C6	6.17	120.08	117.00
1	2A	56	A	N1-C6-N6	-6.17	114.90	118.60
1	2A	2440	C	N3-C4-C5	-6.17	119.43	121.90
32	2a	487	A	N1-C6-N6	6.17	122.30	118.60
1	1A	574	C	N1-C2-O2	6.17	122.60	118.90
1	1A	623	G	C5-C6-O6	-6.17	124.90	128.60
1	1A	1320	C	C4-C5-C6	6.17	120.48	117.40
1	1A	2111	C	C6-N1-C2	-6.17	117.83	120.30
1	1A	517	C	OP2-P-O3'	6.17	118.76	105.20
1	1A	526	A	O5'-P-OP1	-6.17	100.15	105.70
1	1A	1809	A	C5-C6-N1	6.17	120.78	117.70
32	1a	572	A	N7-C8-N9	-6.17	110.72	113.80
32	1a	714	G	OP2-P-O3'	6.17	118.77	105.20
1	2A	807	U	N1-C2-O2	-6.17	118.48	122.80
1	2A	1846	G	C5-C6-N1	-6.17	108.42	111.50
1	2A	2463	C	C6-N1-C2	6.17	122.77	120.30
32	2a	329	A	C4-C5-C6	6.17	120.08	117.00
1	1A	954	G	N1-C6-O6	-6.17	116.20	119.90
32	1a	794	A	OP1-P-OP2	6.17	128.85	119.60
32	2a	1162	C	C6-N1-C2	-6.17	117.83	120.30
1	1A	2239	G	C6-N1-C2	-6.16	121.40	125.10
32	1a	353	A	N1-C6-N6	6.16	122.30	118.60
1	2A	1793	C	C2-N3-C4	-6.16	116.82	119.90
32	2a	853	G	C8-N9-C4	-6.16	103.93	106.40
1	1A	831	G	OP1-P-OP2	-6.16	110.36	119.60
1	1A	2741	A	C5-C6-N1	-6.16	114.62	117.70
1	2A	1777	U	C4-C5-C6	6.16	123.40	119.70
1	1A	1937	A	C2-N3-C4	-6.16	107.52	110.60
1	1A	1996	C	N3-C4-C5	6.16	124.36	121.90
1	1A	2004	G	OP2-P-O3'	6.16	118.75	105.20
1	1A	2502	G	C5-N7-C8	-6.16	101.22	104.30
1	2A	193	U	N3-C4-C5	-6.16	110.90	114.60
4	2E	13	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	1A	765	G	N1-C6-O6	6.16	123.59	119.90
1	1A	1348	G	C5-C6-O6	-6.16	124.91	128.60
1	2A	392	C	N3-C4-N4	-6.16	113.69	118.00
1	2A	1560	G	N3-C4-C5	6.16	131.68	128.60
1	2A	2002	G	C8-N9-C4	6.16	108.86	106.40
1	2A	2478	A	C2-N3-C4	-6.16	107.52	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1137	G	C5-N7-C8	-6.16	101.22	104.30
1	1A	1627	G	OP2-P-O3'	6.16	118.74	105.20
1	1A	2080	G	C8-N9-C4	6.16	108.86	106.40
1	2A	2623	G	C2-N3-C4	6.16	114.98	111.90
1	1A	2683	C	C6-N1-C2	-6.15	117.84	120.30
1	1A	86	C	OP2-P-O3'	6.15	118.73	105.20
1	1A	920	G	OP1-P-OP2	-6.15	110.37	119.60
1	1A	1330	C	C6-N1-C2	6.15	122.76	120.30
1	1A	2008	C	OP1-P-OP2	-6.15	110.37	119.60
1	1A	2315	G	C4-C5-N7	6.15	113.26	110.80
1	1A	2451	A	C2-N3-C4	6.15	113.68	110.60
1	2A	1673	U	C5-C6-N1	-6.15	119.62	122.70
1	2A	2033	A	C6-N1-C2	-6.15	114.91	118.60
1	1A	391	G	C6-C5-N7	-6.15	126.71	130.40
1	1A	1847	A	N7-C8-N9	6.15	116.88	113.80
1	1A	2404	C	N3-C4-N4	-6.15	113.69	118.00
1	1A	2609	U	O5'-P-OP2	-6.15	100.16	105.70
32	1a	353	A	C4-C5-N7	6.15	113.78	110.70
32	1a	1521	G	C5-C6-O6	-6.15	124.91	128.60
1	2A	34	C	C2-N3-C4	6.15	122.97	119.90
1	2A	1721	G	C2-N3-C4	6.15	114.97	111.90
1	1A	2033	A	C8-N9-C4	-6.15	103.34	105.80
32	1a	660	G	N1-C6-O6	6.15	123.59	119.90
1	2A	459	U	N3-C4-O4	-6.15	115.10	119.40
1	2A	2493	U	C5-C6-N1	-6.15	119.62	122.70
1	1A	299	A	OP1-P-O3'	-6.15	91.68	105.20
1	2A	906	G	C6-C5-N7	6.15	134.09	130.40
1	2A	2111	C	N3-C4-C5	-6.15	119.44	121.90
1	1A	869	G	C5-C6-O6	6.15	132.29	128.60
1	2A	2439	A	N9-C4-C5	-6.15	103.34	105.80
1	2A	2468	G	C2-N3-C4	-6.15	108.83	111.90
32	2a	1509	C	C6-N1-C2	6.15	122.76	120.30
32	2a	1523	G	C8-N9-C4	-6.15	103.94	106.40
1	1A	1705	G	N1-C2-N2	-6.14	110.67	116.20
1	1A	1786	A	O4'-C1'-N9	6.14	113.12	108.20
2	1B	56	G	O5'-P-OP2	-6.14	100.17	105.70
32	1a	187	C	C2-N1-C1'	6.14	125.56	118.80
1	2A	869	G	OP1-P-O3'	6.14	118.72	105.20
1	2A	1689	A	C2-N3-C4	-6.14	107.53	110.60
1	1A	484	C	O5'-P-OP1	6.14	118.07	110.70
1	1A	2081	C	OP1-P-OP2	6.14	128.81	119.60
1	1A	2342	C	O5'-P-OP2	6.14	118.07	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	311	A	C8-N9-C4	-6.14	103.34	105.80
1	2A	2102	U	N3-C2-O2	-6.14	117.90	122.20
1	2A	2148	G	C8-N9-C1'	6.14	134.99	127.00
1	1A	521	G	O5'-P-OP1	-6.14	100.17	105.70
1	1A	947	G	C8-N9-C4	-6.14	103.94	106.40
1	1A	993	G	C8-N9-C4	6.14	108.86	106.40
1	2A	794	G	N7-C8-N9	-6.14	110.03	113.10
1	1A	679	C	C2-N3-C4	-6.14	116.83	119.90
1	1A	850	C	O5'-P-OP1	6.14	118.07	110.70
1	1A	1338	G	O5'-P-OP2	-6.14	100.17	105.70
1	1A	1722	A	C8-N9-C4	6.14	108.25	105.80
1	1A	2438	U	C4-C5-C6	6.14	123.38	119.70
1	2A	2231	C	C5-C6-N1	-6.14	117.93	121.00
1	1A	1399	C	C6-N1-C2	6.14	122.75	120.30
1	1A	2487	G	N9-C4-C5	-6.14	102.94	105.40
32	1a	1035	A	C8-N9-C4	-6.14	103.34	105.80
1	2A	1632	A	C5-N7-C8	6.14	106.97	103.90
1	2A	2513	G	C4-C5-N7	6.14	113.25	110.80
1	1A	2235	G	C5-C6-N1	-6.14	108.43	111.50
32	1a	1495	U	N3-C2-O2	-6.14	117.91	122.20
32	2a	1136	U	O4'-C1'-N1	6.14	113.11	108.20
1	2A	381	G	O5'-P-OP2	-6.13	100.18	105.70
1	2A	1804	C	OP1-P-O3'	6.13	118.69	105.20
32	2a	1507	A	C8-N9-C4	6.13	108.25	105.80
1	1A	1281	G	O5'-P-OP2	6.13	118.06	110.70
1	1A	2066	C	C4-C5-C6	-6.13	114.33	117.40
1	2A	989	G	N1-C6-O6	6.13	123.58	119.90
1	1A	416	C	C2-N1-C1'	-6.13	112.06	118.80
1	1A	2033	A	N1-C2-N3	6.13	132.37	129.30
1	1A	2282	G	OP2-P-O3'	6.13	118.69	105.20
32	1a	523	A	N1-C6-N6	6.13	122.28	118.60
1	1A	2004	G	O5'-P-OP1	-6.13	100.18	105.70
32	1a	1065	U	P-O3'-C3'	6.13	127.06	119.70
1	1A	17	G	N3-C4-C5	-6.13	125.54	128.60
1	1A	1158	C	N3-C2-O2	-6.13	117.61	121.90
1	1A	1319	G	OP2-P-O3'	6.13	118.68	105.20
1	1A	1885	A	C8-N9-C4	6.13	108.25	105.80
32	1a	813	U	C6-N1-C2	6.13	124.68	121.00
1	2A	97	C	C2-N1-C1'	-6.13	112.06	118.80
1	2A	1120	G	N7-C8-N9	-6.13	110.04	113.10
1	2A	1678	G	C4-C5-N7	6.13	113.25	110.80
10	2O	8	LEU	CA-CB-CG	6.13	129.40	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1100	C	O4'-C1'-N1	6.13	113.10	108.20
1	1A	2388	A	C4-C5-N7	-6.13	107.64	110.70
1	2A	213	A	C6-C5-N7	6.13	136.59	132.30
1	2A	1297	C	OP2-P-O3'	-6.13	91.72	105.20
1	2A	2423	U	C6-N1-C2	6.13	124.68	121.00
32	2a	656	C	C6-N1-C2	-6.13	117.85	120.30
1	1A	16	G	N3-C2-N2	-6.12	115.61	119.90
1	1A	1265	A	OP1-P-O3'	6.12	118.67	105.20
1	1A	2390	U	C5-C6-N1	6.12	125.76	122.70
1	1A	2609	U	C6-N1-C2	6.12	124.67	121.00
32	1a	1480	G	N3-C4-C5	6.12	131.66	128.60
1	2A	330	A	C4-N9-C1'	6.12	137.33	126.30
1	2A	659	C	C5-C6-N1	-6.12	117.94	121.00
1	2A	2590	A	C5-C6-N1	6.12	120.76	117.70
32	2a	172	A	C8-N9-C4	-6.12	103.35	105.80
1	1A	1003	G	C8-N9-C1'	-6.12	119.04	127.00
1	1A	1266	G	C5-C6-N1	6.12	114.56	111.50
1	1A	1661	G	N7-C8-N9	-6.12	110.04	113.10
1	2A	222	A	C8-N9-C4	6.12	108.25	105.80
1	1A	416	C	C5-C6-N1	-6.12	117.94	121.00
1	1A	1255	U	C2-N1-C1'	6.12	125.05	117.70
1	1A	2026	C	C2-N1-C1'	-6.12	112.07	118.80
1	1A	2548	G	N9-C4-C5	6.12	107.85	105.40
1	2A	330	A	N7-C8-N9	6.12	116.86	113.80
1	2A	1065	U	C5-C6-N1	-6.12	119.64	122.70
1	2A	2439	A	OP1-P-O3'	6.12	118.67	105.20
32	2a	715	A	C2-N3-C4	-6.12	107.54	110.60
32	2a	890	G	O4'-C1'-N9	6.12	113.10	108.20
1	1A	2891	G	C8-N9-C4	6.12	108.85	106.40
1	2A	1283	G	C2-N3-C4	6.12	114.96	111.90
1	2A	1618	A	N1-C6-N6	-6.12	114.93	118.60
1	1A	463	G	C5-C6-N1	-6.12	108.44	111.50
1	1A	1047	G	C8-N9-C1'	-6.12	119.05	127.00
1	1A	2193	G	N7-C8-N9	-6.12	110.04	113.10
32	2a	122	G	N3-C4-N9	6.12	129.67	126.00
1	1A	1231	G	N9-C4-C5	6.12	107.85	105.40
1	1A	1810	A	N1-C6-N6	6.12	122.27	118.60
1	1A	2654	A	N1-C6-N6	6.12	122.27	118.60
32	1a	652	U	C5-C4-O4	-6.12	122.23	125.90
1	2A	2517	C	O5'-P-OP1	-6.12	100.20	105.70
1	1A	510	C	N1-C2-O2	-6.11	115.23	118.90
1	1A	583	G	OP1-P-O3'	6.11	118.65	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	148	G	N3-C4-C5	-6.11	125.54	128.60
32	1a	801	U	C6-N1-C2	6.11	124.67	121.00
1	1A	1612	C	O5'-P-OP2	-6.11	100.20	105.70
9	1N	85	ILE	CB-CA-C	-6.11	99.38	111.60
1	1A	766	C	N3-C4-C5	6.11	124.34	121.90
1	1A	938	G	O5'-P-OP1	6.11	118.03	110.70
1	1A	1839	G	N9-C4-C5	-6.11	102.95	105.40
1	1A	2249	U	C4-C5-C6	-6.11	116.03	119.70
32	1a	181	G	C8-N9-C4	-6.11	103.96	106.40
1	2A	1029	A	C5-C6-N6	-6.11	118.81	123.70
1	2A	1073	A	C5-C6-N6	6.11	128.59	123.70
1	1A	1606	G	N1-C2-N3	6.11	127.56	123.90
1	2A	330	A	N1-C6-N6	6.11	122.26	118.60
1	2A	462	C	N3-C4-N4	-6.11	113.72	118.00
1	2A	2005	A	C6-N1-C2	-6.11	114.94	118.60
1	2A	2700	C	C5-C6-N1	-6.11	117.95	121.00
2	2B	20	C	C6-N1-C2	6.11	122.74	120.30
23	2I	21	ARG	NE-CZ-NH2	-6.11	117.25	120.30
32	2a	789	U	C5-C4-O4	6.11	129.56	125.90
1	1A	791	C	N3-C4-N4	6.11	122.27	118.00
1	1A	1965	C	O5'-P-OP1	-6.11	100.20	105.70
1	1A	2038	G	C8-N9-C4	-6.11	103.96	106.40
1	1A	2780	G	N9-C4-C5	6.11	107.84	105.40
1	1A	2886	G	N3-C2-N2	-6.11	115.63	119.90
32	1a	1106	G	C8-N9-C4	-6.11	103.96	106.40
1	2A	2018	G	C5-C6-O6	-6.11	124.94	128.60
1	2A	2328	A	N1-C6-N6	6.11	122.26	118.60
1	1A	528	A	N3-C4-C5	-6.10	122.53	126.80
1	1A	1274	A	C4-C5-C6	6.10	120.05	117.00
1	1A	1790	C	OP1-P-O3'	6.10	118.63	105.20
1	1A	712	G	C4-C5-N7	6.10	113.24	110.80
1	1A	1648	C	N3-C4-C5	6.10	124.34	121.90
9	1N	74	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	2A	1047	G	C4-N9-C1'	6.10	134.43	126.50
1	2A	2595	G	C2-N3-C4	-6.10	108.85	111.90
1	2A	2855	C	C6-N1-C2	-6.10	117.86	120.30
32	2a	22	G	N1-C6-O6	6.10	123.56	119.90
1	1A	1812	A	C6-N1-C2	-6.10	114.94	118.60
2	1B	104	U	C5-C6-N1	-6.10	119.65	122.70
1	1A	807	U	C5-C4-O4	-6.10	122.24	125.90
1	1A	1576	U	C5-C4-O4	6.10	129.56	125.90
1	1A	2294	C	C6-N1-C2	-6.10	117.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	376	G	N7-C8-N9	-6.10	110.05	113.10
1	2A	171	G	O4'-C1'-N9	6.10	113.08	108.20
2	2B	117	G	C2-N3-C4	-6.10	108.85	111.90
1	1A	962	G	OP1-P-OP2	-6.10	110.45	119.60
1	1A	1669	A	O4'-C1'-N9	6.10	113.08	108.20
1	1A	2062	A	C5-C6-N6	-6.10	118.82	123.70
1	1A	2829	C	C5-C4-N4	-6.10	115.93	120.20
1	2A	311	A	OP1-P-OP2	-6.10	110.45	119.60
1	2A	1678	G	C8-N9-C1'	-6.10	119.07	127.00
1	2A	1692	U	N3-C4-O4	6.10	123.67	119.40
1	1A	763	G	C5-C6-N1	-6.10	108.45	111.50
1	1A	2063	C	N3-C2-O2	6.10	126.17	121.90
32	1a	613	C	C6-N1-C2	-6.10	117.86	120.30
1	2A	646	A	C5-C6-N1	-6.10	114.65	117.70
1	2A	1639	U	N1-C2-N3	6.10	118.56	114.90
1	2A	2140	C	C6-N1-C2	-6.10	117.86	120.30
1	1A	197	A	C2-N3-C4	-6.09	107.55	110.60
1	1A	203	C	C5-C6-N1	-6.09	117.95	121.00
1	1A	1566	A	C4-C5-N7	-6.09	107.65	110.70
1	1A	2116	G	C4-N9-C1'	6.09	134.42	126.50
1	1A	2685	G	C5-C6-O6	6.09	132.26	128.60
1	2A	2334	G	C8-N9-C4	6.09	108.84	106.40
1	2A	2808	U	N1-C2-N3	-6.09	111.24	114.90
1	1A	2242	G	N3-C2-N2	-6.09	115.64	119.90
32	1a	633	G	N3-C4-C5	6.09	131.65	128.60
1	2A	576	U	OP1-P-OP2	6.09	128.74	119.60
1	1A	338	G	N1-C2-N3	6.09	127.56	123.90
1	1A	1653	G	C5-C6-N1	-6.09	108.45	111.50
1	1A	1196	C	C2-N3-C4	-6.09	116.86	119.90
1	1A	1841	U	O5'-P-OP2	-6.09	100.22	105.70
32	1a	564	C	C6-N1-C2	6.09	122.74	120.30
1	2A	1826	G	N7-C8-N9	-6.09	110.06	113.10
1	2A	2562	U	N3-C4-O4	6.09	123.66	119.40
32	1a	1442	G	N3-C4-C5	-6.09	125.56	128.60
1	1A	2512	C	C6-N1-C2	6.09	122.73	120.30
32	1a	1412	C	C5-C6-N1	-6.09	117.96	121.00
1	2A	1331	A	N9-C4-C5	6.09	108.23	105.80
1	1A	997	G	C4-C5-N7	-6.08	108.37	110.80
32	1a	172	A	C8-N9-C4	-6.08	103.37	105.80
1	1A	290	G	N3-C2-N2	6.08	124.16	119.90
1	1A	476	G	N9-C4-C5	-6.08	102.97	105.40
1	1A	1514	U	C5-C6-N1	-6.08	119.66	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2472	G	C5-C6-O6	-6.08	124.95	128.60
1	2A	508	G	O5'-P-OP1	-6.08	100.23	105.70
1	1A	117	G	C8-N9-C4	6.08	108.83	106.40
1	1A	376	C	C6-N1-C2	6.08	122.73	120.30
1	1A	1546	C	O5'-P-OP2	6.08	118.00	110.70
1	1A	2397	G	N3-C2-N2	-6.08	115.64	119.90
1	2A	945	A	N9-C4-C5	-6.08	103.37	105.80
1	2A	1671	U	C6-N1-C2	6.08	124.65	121.00
32	2a	1202	G	C4-C5-N7	-6.08	108.37	110.80
1	1A	426	C	O5'-P-OP1	-6.08	100.23	105.70
1	1A	2590	A	N1-C6-N6	6.08	122.25	118.60
1	2A	860	U	N3-C2-O2	-6.08	117.94	122.20
1	2A	1205	U	C6-N1-C2	-6.08	117.35	121.00
1	1A	724	U	C5-C6-N1	-6.08	119.66	122.70
1	1A	990	A	N7-C8-N9	6.08	116.84	113.80
2	1B	68	C	OP2-P-O3'	6.08	118.57	105.20
1	2A	739	G	O5'-P-OP1	-6.08	100.23	105.70
1	2A	1021	A	N7-C8-N9	6.08	116.84	113.80
1	1A	770	G	C2-N3-C4	-6.08	108.86	111.90
1	1A	777	A	C6-N1-C2	-6.08	114.95	118.60
1	1A	2860	A	OP2-P-O3'	6.08	118.56	105.20
1	2A	134	C	C6-N1-C2	6.08	122.73	120.30
1	2A	693	C	C2-N1-C1'	-6.08	112.12	118.80
1	2A	2280	G	N3-C4-C5	6.08	131.64	128.60
1	2A	2378	A	C5-C6-N1	-6.08	114.66	117.70
1	1A	16	G	OP1-P-O3'	6.07	118.56	105.20
1	1A	133	C	O5'-P-OP1	6.07	117.99	110.70
1	1A	604	G	C2-N3-C4	-6.07	108.86	111.90
1	1A	606	U	O5'-P-OP2	-6.07	100.23	105.70
1	1A	1982	C	C5-C6-N1	6.07	124.04	121.00
32	2a	59	A	N1-C6-N6	6.07	122.24	118.60
32	1a	1270	C	N1-C2-O2	6.07	122.54	118.90
1	2A	1793	C	N3-C4-N4	-6.07	113.75	118.00
1	1A	2613	U	C5-C4-O4	6.07	129.54	125.90
1	1A	2627	G	N9-C4-C5	-6.07	102.97	105.40
2	1B	13	A	C8-N9-C4	6.07	108.23	105.80
32	1a	491	G	C8-N9-C1'	6.07	134.89	127.00
1	2A	496	G	C8-N9-C4	-6.07	103.97	106.40
1	2A	754	C	N3-C4-N4	6.07	122.25	118.00
1	2A	1328	G	C8-N9-C4	6.07	108.83	106.40
1	1A	2442	C	C4-C5-C6	6.07	120.44	117.40
9	1N	25	ARG	NE-CZ-NH1	-6.07	117.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1P	15	ARG	NE-CZ-NH2	6.07	123.33	120.30
32	1a	427	U	N1-C2-O2	6.07	127.05	122.80
1	2A	245	G	C4-N9-C1'	6.07	134.39	126.50
32	2a	357	G	C4-C5-N7	-6.07	108.37	110.80
1	1A	203	C	C2-N1-C1'	-6.07	112.13	118.80
1	1A	2082	A	N7-C8-N9	-6.07	110.77	113.80
2	1B	104	U	C6-N1-C2	6.07	124.64	121.00
1	2A	501	A	C2-N3-C4	-6.07	107.57	110.60
1	2A	2223	G	O5'-P-OP1	6.07	117.98	110.70
32	2a	1016	A	N1-C6-N6	6.07	122.24	118.60
32	2a	1406	U	C2-N3-C4	-6.07	123.36	127.00
1	1A	751	A	C5-C6-N1	6.06	120.73	117.70
1	1A	1638	C	OP2-P-O3'	6.06	118.54	105.20
1	1A	1683	C	C5-C6-N1	-6.06	117.97	121.00
1	1A	1955	U	C6-N1-C2	6.06	124.64	121.00
1	1A	2149	G	C8-N9-C4	6.06	108.83	106.40
1	1A	1202	C	N1-C2-O2	-6.06	115.26	118.90
1	2A	1256	G	O5'-P-OP2	-6.06	100.24	105.70
2	2B	24	G	C4-C5-N7	6.06	113.22	110.80
32	2a	815	A	N7-C8-N9	-6.06	110.77	113.80
32	1a	150	C	C6-N1-C2	-6.06	117.88	120.30
1	1A	140	G	C2-N3-C4	-6.06	108.87	111.90
1	1A	1217	C	N3-C4-N4	6.06	122.24	118.00
1	1A	1552	G	C5-C6-N1	6.06	114.53	111.50
1	2A	446	G	C2-N3-C4	-6.06	108.87	111.90
1	2A	470	A	N9-C4-C5	-6.06	103.38	105.80
1	2A	988	A	C6-C5-N7	-6.06	128.06	132.30
1	2A	2191	G	C6-C5-N7	-6.06	126.76	130.40
1	2A	2492	U	OP1-P-OP2	-6.06	110.51	119.60
1	1A	215	G	C5-C6-N1	-6.06	108.47	111.50
1	1A	988	A	N9-C4-C5	-6.06	103.38	105.80
1	1A	1349	A	O5'-P-OP2	-6.06	100.25	105.70
1	1A	2041	U	OP1-P-O3'	-6.06	91.87	105.20
1	1A	2390	U	C6-N1-C2	-6.06	117.36	121.00
1	1A	2689	U	P-O3'-C3'	6.06	126.97	119.70
1	1A	2773	C	N3-C4-N4	6.06	122.24	118.00
1	2A	1327	C	C6-N1-C2	-6.06	117.88	120.30
1	1A	2424	C	C2-N1-C1'	-6.06	112.14	118.80
1	2A	1252	G	C8-N9-C4	6.06	108.82	106.40
1	2A	1562	A	N1-C6-N6	6.06	122.23	118.60
1	1A	261	G	N3-C4-C5	6.05	131.63	128.60
1	1A	912	C	N3-C2-O2	-6.05	117.66	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	974	G	N9-C4-C5	6.05	107.82	105.40
1	1A	1319	G	N7-C8-N9	6.05	116.13	113.10
32	1a	1493	A	N7-C8-N9	6.05	116.83	113.80
1	2A	1325	G	C8-N9-C1'	-6.05	119.13	127.00
32	2a	1067	A	P-O3'-C3'	6.05	126.97	119.70
32	2a	1509	C	C5-C6-N1	-6.05	117.97	121.00
1	1A	1186	G	N1-C2-N3	6.05	127.53	123.90
1	1A	1440	G	C8-N9-C4	6.05	108.82	106.40
32	1a	1500	A	N1-C6-N6	6.05	122.23	118.60
1	2A	589	C	C5-C6-N1	6.05	124.03	121.00
1	2A	1602	U	O5'-P-OP2	6.05	117.96	110.70
32	1a	1058	G	N9-C4-C5	-6.05	102.98	105.40
1	2A	561	G	C6-C5-N7	-6.05	126.77	130.40
1	2A	1175	U	OP1-P-O3'	6.05	118.52	105.20
1	2A	2047	U	N3-C4-O4	-6.05	115.16	119.40
1	2A	2620	C	C5-C4-N4	-6.05	115.96	120.20
2	2B	64	C	C6-N1-C2	6.05	122.72	120.30
32	2a	1126	U	C2-N1-C1'	6.05	124.96	117.70
1	1A	988	A	OP2-P-O3'	6.05	118.51	105.20
1	1A	1137	G	C4-C5-N7	6.05	113.22	110.80
2	2B	74	U	N1-C2-N3	6.05	118.53	114.90
1	1A	61	G	N3-C2-N2	-6.05	115.67	119.90
1	1A	1577	C	N1-C2-O2	6.05	122.53	118.90
1	1A	1633	G	N1-C6-O6	-6.05	116.27	119.90
1	2A	2058	A	C4-C5-C6	6.05	120.02	117.00
1	1A	1194	A	C6-N1-C2	-6.05	114.97	118.60
1	1A	1632	A	C2-N3-C4	-6.05	107.58	110.60
1	1A	2283	C	N1-C2-N3	-6.05	114.97	119.20
1	1A	2803	C	C6-N1-C2	-6.05	117.88	120.30
1	2A	1403	C	N3-C2-O2	-6.05	117.67	121.90
1	2A	2755	C	C6-N1-C2	-6.05	117.88	120.30
1	1A	136	G	C2-N3-C4	-6.04	108.88	111.90
1	1A	2834	G	C4-C5-N7	-6.04	108.38	110.80
32	1a	1442	G	C6-C5-N7	-6.04	126.77	130.40
1	2A	2721	A	N1-C2-N3	6.04	132.32	129.30
1	1A	180	G	C5-C6-N1	6.04	114.52	111.50
1	1A	1774	C	C6-N1-C2	6.04	122.72	120.30
1	2A	238	C	N3-C4-C5	-6.04	119.48	121.90
1	2A	1065	U	C2-N3-C4	-6.04	123.38	127.00
1	2A	1597	A	C8-N9-C4	6.04	108.22	105.80
1	1A	1220	A	N1-C6-N6	-6.04	114.98	118.60
1	2A	740	U	OP1-P-O3'	6.04	118.49	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1770	G	C6-C5-N7	6.04	134.02	130.40
1	1A	2116	G	C8-N9-C4	-6.04	103.98	106.40
32	2a	748	C	C2-N1-C1'	-6.04	112.16	118.80
32	2a	799	G	N1-C6-O6	-6.04	116.28	119.90
32	2a	856	C	N3-C4-C5	-6.04	119.48	121.90
1	1A	790	C	N1-C2-O2	-6.04	115.28	118.90
1	1A	1799	G	N7-C8-N9	-6.04	110.08	113.10
1	1A	2476	A	OP1-P-OP2	6.04	128.65	119.60
1	1A	2587	A	OP1-P-O3'	6.04	118.48	105.20
32	1a	912	C	N3-C2-O2	6.04	126.12	121.90
32	1a	1087	G	N3-C4-C5	-6.04	125.58	128.60
1	1A	32	C	N3-C2-O2	6.03	126.12	121.90
1	1A	1304	C	C4-C5-C6	-6.03	114.38	117.40
1	1A	2393	A	N9-C4-C5	6.03	108.21	105.80
1	2A	825	C	OP2-P-O3'	6.03	118.47	105.20
1	1A	1252	G	O4'-C1'-N9	-6.03	103.37	108.20
1	1A	432	A	C4-C5-C6	6.03	120.02	117.00
1	1A	457	A	OP1-P-OP2	-6.03	110.55	119.60
1	1A	1839	G	OP1-P-OP2	6.03	128.65	119.60
1	1A	2032	G	N7-C8-N9	-6.03	110.08	113.10
1	1A	2076	U	N1-C2-N3	6.03	118.52	114.90
1	1A	2466	C	N3-C2-O2	6.03	126.12	121.90
1	1A	2565	A	OP2-P-O3'	6.03	118.47	105.20
1	2A	521	G	C6-C5-N7	-6.03	126.78	130.40
1	2A	530	G	O5'-P-OP2	6.03	117.94	110.70
1	2A	2859	G	N3-C4-C5	-6.03	125.58	128.60
1	1A	2430	A	N7-C8-N9	6.03	116.81	113.80
1	2A	1388	G	C8-N9-C4	6.03	108.81	106.40
1	1A	215	G	OP1-P-OP2	-6.03	110.56	119.60
1	1A	743	G	C8-N9-C4	-6.03	103.99	106.40
1	1A	1125	G	N1-C2-N2	-6.03	110.78	116.20
1	2A	1205	U	N3-C2-O2	-6.03	117.98	122.20
1	2A	2446	G	N1-C2-N2	-6.03	110.78	116.20
32	2a	533	A	C6-C5-N7	-6.03	128.08	132.30
32	2a	550	G	C8-N9-C4	6.03	108.81	106.40
1	1A	132	G	N7-C8-N9	-6.03	110.09	113.10
1	1A	626	U	OP1-P-O3'	6.03	118.45	105.20
1	1A	1655	A	C4-C5-N7	6.03	113.71	110.70
1	1A	2377	A	N1-C6-N6	6.03	122.22	118.60
1	1A	2609	U	C4-C5-C6	6.03	123.31	119.70
1	1A	2627	G	O5'-P-OP2	-6.03	100.28	105.70
1	2A	1996	C	O5'-P-OP1	-6.03	100.28	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2391	G	N9-C4-C5	-6.03	102.99	105.40
1	1A	74	A	OP1-P-OP2	-6.02	110.56	119.60
1	1A	901	A	N1-C6-N6	6.02	122.22	118.60
1	2A	764	A	N7-C8-N9	6.02	116.81	113.80
1	1A	870	A	C2-N3-C4	-6.02	107.59	110.60
1	1A	1476	C	N1-C2-O2	-6.02	115.29	118.90
32	1a	1466	C	C5-C4-N4	6.02	124.42	120.20
1	2A	959	A	C4-N9-C1'	6.02	137.14	126.30
32	2a	1528	U	C6-N1-C2	6.02	124.61	121.00
1	1A	1018	C	N1-C2-N3	-6.02	114.99	119.20
1	2A	86	C	C6-N1-C2	6.02	122.71	120.30
1	2A	1416	G	N7-C8-N9	-6.02	110.09	113.10
1	2A	1496	A	C8-N9-C4	-6.02	103.39	105.80
1	2A	1629	U	N3-C4-C5	-6.02	110.99	114.60
1	2A	2630	G	N3-C4-N9	-6.02	122.39	126.00
32	2a	28	G	N1-C6-O6	6.02	123.51	119.90
32	2a	893	C	C5-C6-N1	-6.02	117.99	121.00
34	2c	91	LEU	CA-CB-CG	6.02	129.15	115.30
1	1A	1361	G	C5-C6-N1	6.02	114.51	111.50
1	1A	1627	G	C2-N3-C4	6.02	114.91	111.90
1	1A	2025	C	OP1-P-O3'	-6.02	91.96	105.20
1	2A	207	A	C4-C5-C6	6.02	120.01	117.00
1	2A	818	G	N3-C4-C5	6.02	131.61	128.60
1	2A	1120	G	N3-C4-C5	6.02	131.61	128.60
32	2a	841	U	N3-C2-O2	-6.02	117.99	122.20
1	1A	330	A	N3-C4-C5	6.02	131.01	126.80
32	2a	487	A	N9-C4-C5	-6.02	103.39	105.80
1	1A	652(S)	C	C5-C6-N1	6.01	124.01	121.00
2	1B	62	C	C6-N1-C2	6.01	122.71	120.30
1	2A	699	A	O5'-P-OP1	-6.01	100.29	105.70
1	2A	1935	G	C4-C5-N7	6.01	113.21	110.80
1	2A	2357	U	N1-C2-O2	6.01	127.01	122.80
32	2a	49	U	C6-N1-C2	6.01	124.61	121.00
1	2A	630	G	N7-C8-N9	-6.01	110.09	113.10
1	2A	792	G	N3-C4-N9	6.01	129.61	126.00
1	2A	873	G	C8-N9-C4	6.01	108.81	106.40
1	1A	860	U	O5'-P-OP1	6.01	117.92	110.70
1	1A	956	G	N1-C6-O6	6.01	123.51	119.90
1	1A	2071	A	O5'-P-OP2	-6.01	100.29	105.70
1	2A	58	G	C6-C5-N7	-6.01	126.79	130.40
1	2A	197	A	N1-C6-N6	6.01	122.21	118.60
1	2A	597	U	N3-C2-O2	6.01	126.41	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1372	U	C5-C6-N1	6.01	125.70	122.70
1	1A	74	A	N1-C6-N6	-6.01	114.99	118.60
1	1A	1185	C	O5'-P-OP1	-6.01	100.29	105.70
1	1A	1799	G	N9-C4-C5	-6.01	103.00	105.40
1	2A	329	G	N3-C4-N9	6.01	129.61	126.00
1	2A	1315	C	O5'-P-OP2	-6.01	100.29	105.70
1	2A	1788	C	O5'-P-OP1	-6.01	100.29	105.70
1	2A	2297	C	C2-N1-C1'	-6.01	112.19	118.80
1	1A	318	C	C6-N1-C2	-6.01	117.90	120.30
1	2A	468	G	C5-C6-O6	-6.01	125.00	128.60
1	2A	1212	G	C8-N9-C4	6.01	108.80	106.40
1	2A	1409	C	OP1-P-OP2	6.01	128.61	119.60
1	1A	2023	G	O5'-P-OP2	6.01	117.91	110.70
1	1A	2758	A	C5-C6-N6	-6.01	118.89	123.70
1	2A	425	G	O5'-P-OP2	-6.01	100.29	105.70
1	2A	505	A	N1-C6-N6	6.01	122.20	118.60
1	2A	759	G	N1-C6-O6	6.01	123.50	119.90
32	2a	975	A	O4'-C1'-N9	-6.01	103.39	108.20
1	2A	2191	G	N3-C4-N9	6.00	129.60	126.00
1	1A	248	G	N1-C6-O6	-6.00	116.30	119.90
1	1A	2111	C	C5-C6-N1	6.00	124.00	121.00
1	2A	177	G	N3-C4-N9	-6.00	122.40	126.00
1	1A	103	A	N9-C4-C5	-6.00	103.40	105.80
1	1A	476	G	C5-C6-O6	-6.00	125.00	128.60
1	1A	734	A	C2-N3-C4	-6.00	107.60	110.60
1	1A	2570	G	O5'-P-OP2	-6.00	100.30	105.70
1	1A	2746	U	C2-N1-C1'	-6.00	110.50	117.70
1	1A	1072	C	C6-N1-C2	-6.00	117.90	120.30
1	2A	2243	U	N3-C2-O2	6.00	126.40	122.20
1	1A	598	G	OP1-P-OP2	6.00	128.60	119.60
1	1A	998	C	N1-C2-O2	-6.00	115.30	118.90
1	2A	2430	A	O5'-P-OP2	-6.00	100.30	105.70
1	1A	572	A	N7-C8-N9	6.00	116.80	113.80
1	1A	1304	C	C2-N1-C1'	-6.00	112.20	118.80
1	2A	409	C	N3-C2-O2	6.00	126.10	121.90
1	2A	1997	G	OP2-P-O3'	6.00	118.39	105.20
32	2a	543	C	N3-C4-C5	-6.00	119.50	121.90
1	1A	1819	A	C5-C6-N1	-6.00	114.70	117.70
1	1A	2860	A	C8-N9-C4	5.99	108.20	105.80
1	2A	187	G	C5-C6-O6	-5.99	125.00	128.60
1	2A	271(X)	G	C5-C6-N1	-5.99	108.50	111.50
1	2A	1325	G	C5-C6-O6	-5.99	125.00	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2102	U	C5-C6-N1	5.99	125.70	122.70
1	2A	2321	G	N3-C4-C5	-5.99	125.60	128.60
1	1A	1554	A	C8-N9-C4	5.99	108.20	105.80
1	1A	1721	G	C5-N7-C8	-5.99	101.30	104.30
1	1A	2578	G	N1-C2-N2	5.99	121.59	116.20
1	2A	2004	G	N3-C4-N9	-5.99	122.41	126.00
1	2A	2675	A	O5'-P-OP1	5.99	117.89	110.70
1	1A	128	C	N3-C4-C5	5.99	124.30	121.90
1	1A	622	G	C4-N9-C1'	5.99	134.29	126.50
1	1A	1307	A	C8-N9-C4	5.99	108.20	105.80
1	1A	2440	C	N3-C4-N4	-5.99	113.81	118.00
1	1A	2476	A	C4-N9-C1'	5.99	137.08	126.30
1	1A	2492	U	N3-C2-O2	-5.99	118.01	122.20
1	1A	2517	C	O4'-C1'-N1	5.99	112.99	108.20
1	1A	2825	C	N3-C2-O2	5.99	126.09	121.90
1	2A	994	C	N1-C2-O2	5.99	122.49	118.90
1	2A	2116	G	C8-N9-C4	-5.99	104.00	106.40
1	1A	525	U	O5'-P-OP2	-5.99	100.31	105.70
1	1A	856	C	C2-N3-C4	5.99	122.89	119.90
1	1A	1244	G	C2-N3-C4	-5.99	108.91	111.90
1	1A	2717	G	N9-C4-C5	-5.99	103.00	105.40
32	1a	189(G)	G	N3-C4-C5	5.99	131.59	128.60
1	2A	670	A	C8-N9-C4	5.99	108.19	105.80
1	2A	2191	G	C4-N9-C1'	5.99	134.28	126.50
1	1A	635	C	OP1-P-OP2	5.99	128.58	119.60
1	1A	707	G	N1-C6-O6	5.99	123.49	119.90
21	1Z	86	VAL	CB-CA-C	-5.99	100.02	111.40
32	1a	429	U	O5'-P-OP1	-5.99	100.31	105.70
1	2A	1611	C	N3-C4-N4	5.99	122.19	118.00
1	2A	2468	G	N1-C6-O6	5.99	123.49	119.90
1	1A	671	C	N3-C4-C5	-5.99	119.51	121.90
1	1A	801	G	O5'-P-OP2	-5.99	100.31	105.70
1	1A	1144	G	O5'-P-OP1	5.99	117.88	110.70
1	1A	2005	A	C2-N3-C4	5.99	113.59	110.60
1	2A	2562	U	N1-C2-N3	5.99	118.49	114.90
1	2A	2763	G	N1-C6-O6	5.99	123.49	119.90
1	2A	2832	U	C6-N1-C2	5.99	124.59	121.00
1	1A	463	G	OP1-P-OP2	5.98	128.57	119.60
1	1A	739	G	N1-C6-O6	5.98	123.49	119.90
1	1A	1670	C	C5-C4-N4	5.98	124.39	120.20
1	2A	1349	A	O5'-P-OP1	-5.98	100.31	105.70
1	1A	669	G	N1-C6-O6	5.98	123.49	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	750	A	OP2-P-O3'	5.98	118.36	105.20
32	2a	728	A	N7-C8-N9	5.98	116.79	113.80
32	2a	1028	C	C2-N3-C4	5.98	122.89	119.90
1	1A	1429	G	N3-C4-C5	-5.98	125.61	128.60
32	1a	897	C	C5-C6-N1	-5.98	118.01	121.00
32	1a	1468	A	N1-C6-N6	5.98	122.19	118.60
1	2A	26	G	C6-C5-N7	-5.98	126.81	130.40
1	2A	938	G	C5-C6-N1	-5.98	108.51	111.50
1	2A	979	G	C4-C5-N7	-5.98	108.41	110.80
1	1A	1239	G	C4-C5-N7	5.98	113.19	110.80
1	1A	1659	U	O5'-P-OP2	-5.98	100.32	105.70
1	1A	2265	U	C2-N3-C4	-5.98	123.41	127.00
32	1a	15	G	C6-C5-N7	-5.98	126.81	130.40
1	1A	30	G	O5'-P-OP2	-5.98	100.32	105.70
1	1A	70	G	C8-N9-C4	-5.98	104.01	106.40
1	1A	1130	U	N1-C2-N3	5.98	118.49	114.90
2	1B	84	C	C5-C6-N1	5.98	123.99	121.00
32	1a	954	G	O5'-P-OP2	-5.98	100.32	105.70
1	2A	603	A	N1-C6-N6	5.98	122.19	118.60
1	2A	2378	A	N3-C4-N9	5.98	132.18	127.40
32	1a	1524	C	C2-N3-C4	-5.98	116.91	119.90
32	2a	26	A	O5'-P-OP2	-5.98	100.32	105.70
1	1A	658	C	N3-C4-C5	-5.97	119.51	121.90
1	1A	2206	G	C5-C6-O6	-5.97	125.02	128.60
1	1A	2887	U	O5'-P-OP1	-5.97	100.32	105.70
1	2A	827	U	N3-C4-O4	5.97	123.58	119.40
1	2A	1338	G	C8-N9-C4	-5.97	104.01	106.40
1	2A	2607	G	C6-C5-N7	-5.97	126.81	130.40
1	2A	2874	C	O5'-P-OP2	-5.97	100.32	105.70
1	1A	179	G	C6-C5-N7	-5.97	126.82	130.40
1	1A	532	A	N1-C2-N3	-5.97	126.31	129.30
1	1A	790	C	C2-N1-C1'	5.97	125.37	118.80
1	1A	861	A	N9-C4-C5	-5.97	103.41	105.80
1	1A	1339	G	N7-C8-N9	5.97	116.09	113.10
1	1A	2015	A	N1-C2-N3	5.97	132.29	129.30
32	1a	1406	U	O5'-P-OP1	5.97	117.87	110.70
32	1a	1524	C	C5-C6-N1	-5.97	118.01	121.00
1	2A	465	G	O5'-P-OP2	5.97	117.87	110.70
1	2A	739	G	OP2-P-O3'	-5.97	92.06	105.20
1	2A	2227	A	C2-N3-C4	-5.97	107.61	110.60
1	2A	2319	G	N9-C1'-C2'	5.97	121.76	114.00
1	1A	1703	G	C8-N9-C4	-5.97	104.01	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1773	A	C5-C6-N1	-5.97	114.71	117.70
1	2A	2136	C	C6-N1-C2	-5.97	117.91	120.30
1	1A	865	C	OP1-P-OP2	-5.97	110.65	119.60
1	1A	1206	G	N1-C2-N3	5.97	127.48	123.90
1	1A	1440	G	N7-C8-N9	-5.97	110.11	113.10
1	1A	1901	A	C5-C6-N1	5.97	120.69	117.70
1	1A	2032	G	C6-C5-N7	-5.97	126.82	130.40
32	1a	895	G	N3-C4-N9	-5.97	122.42	126.00
1	2A	58	G	N7-C8-N9	5.97	116.08	113.10
1	2A	2288	A	C5-C6-N6	-5.97	118.92	123.70
32	2a	740	U	C5-C6-N1	-5.97	119.72	122.70
1	1A	1762	A	C8-N9-C4	5.97	108.19	105.80
1	2A	1308	A	C2-N3-C4	-5.97	107.62	110.60
32	1a	529	G	C6-C5-N7	-5.97	126.82	130.40
1	2A	2699	C	C5-C6-N1	-5.97	118.02	121.00
1	1A	837	C	C6-N1-C2	-5.96	117.91	120.30
1	1A	2727	G	OP1-P-OP2	5.96	128.55	119.60
1	1A	2764	A	C5-C6-N6	5.96	128.47	123.70
1	2A	734	A	C5-C6-N1	-5.96	114.72	117.70
1	2A	805	G	C8-N9-C4	-5.96	104.01	106.40
1	2A	1188	U	N1-C2-O2	5.96	126.97	122.80
32	2a	59	A	N9-C4-C5	-5.96	103.42	105.80
1	1A	513	A	N3-C4-C5	-5.96	122.63	126.80
1	1A	726	G	C2-N3-C4	-5.96	108.92	111.90
1	1A	960	A	C5-N7-C8	-5.96	100.92	103.90
1	1A	1231	G	OP1-P-OP2	-5.96	110.66	119.60
32	1a	398	C	N3-C4-C5	5.96	124.28	121.90
32	2a	898	G	C2-N3-C4	-5.96	108.92	111.90
1	1A	1162	G	OP1-P-O3'	5.96	118.31	105.20
1	1A	1379	A	C8-N9-C4	5.96	108.18	105.80
1	1A	2036	C	C5-C4-N4	5.96	124.37	120.20
32	1a	773	G	N3-C4-C5	5.96	131.58	128.60
1	2A	1036	G	N3-C4-C5	5.96	131.58	128.60
1	2A	1633	G	C5-C6-N1	5.96	114.48	111.50
8	2I	38	LEU	CB-CG-CD2	5.96	121.13	111.00
32	2a	415	A	C8-N9-C4	-5.96	103.42	105.80
1	1A	513	A	C4-N9-C1'	5.96	137.03	126.30
1	1A	1565	C	OP2-P-O3'	5.96	118.31	105.20
1	1A	2323	G	C5-C6-O6	-5.96	125.03	128.60
32	1a	831	U	C5-C6-N1	5.96	125.68	122.70
32	1a	1278	U	C2-N1-C1'	5.96	124.85	117.70
1	2A	652(A)	A	C2-N3-C4	5.96	113.58	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1636	C	O5'-P-OP1	-5.96	100.34	105.70
1	1A	242	G	N9-C4-C5	-5.96	103.02	105.40
1	1A	2019	A	C6-C5-N7	-5.96	128.13	132.30
1	1A	2022	U	O5'-P-OP1	-5.96	100.34	105.70
1	1A	2554	U	N3-C4-O4	5.96	123.57	119.40
1	1A	2733	A	C5-N7-C8	-5.96	100.92	103.90
6	2G	82	LEU	CA-CB-CG	5.96	129.00	115.30
32	2a	975	A	C2-N3-C4	-5.96	107.62	110.60
1	1A	773	U	C6-N1-C2	5.96	124.57	121.00
1	1A	83	G	N3-C2-N2	5.95	124.07	119.90
1	1A	95	G	N3-C4-C5	-5.95	125.62	128.60
1	1A	197	A	C5-N7-C8	-5.95	100.92	103.90
1	1A	2419	U	C5-C4-O4	5.95	129.47	125.90
15	1T	53	ARG	CB-CA-C	-5.95	98.49	110.40
32	1a	790	A	C2-N3-C4	-5.95	107.62	110.60
32	1a	1286	A	N1-C6-N6	-5.95	115.03	118.60
32	1a	1384	C	C5-C6-N1	5.95	123.98	121.00
1	1A	742	G	N1-C2-N2	5.95	121.56	116.20
1	1A	2038	G	N3-C4-C5	-5.95	125.62	128.60
32	1a	869	G	O5'-P-OP1	-5.95	100.34	105.70
32	1a	1084	G	N3-C2-N2	5.95	124.07	119.90
32	2a	27	G	N1-C6-O6	5.95	123.47	119.90
32	2a	905	U	N3-C4-C5	-5.95	111.03	114.60
1	1A	423	A	N1-C6-N6	-5.95	115.03	118.60
1	1A	1217	C	O5'-P-OP1	-5.95	100.34	105.70
1	1A	2319	G	N1-C2-N2	-5.95	110.84	116.20
1	2A	20	C	N1-C2-O2	-5.95	115.33	118.90
1	2A	1274	A	C5-N7-C8	-5.95	100.92	103.90
1	1A	79	G	N3-C2-N2	-5.95	115.74	119.90
1	1A	448	U	C4-C5-C6	5.95	123.27	119.70
1	1A	1493	C	N1-C2-O2	5.95	122.47	118.90
1	2A	117	G	C8-N9-C4	-5.95	104.02	106.40
1	2A	185	U	C2-N3-C4	-5.95	123.43	127.00
1	2A	574	C	O5'-P-OP1	-5.95	100.35	105.70
1	2A	607	U	O5'-P-OP2	-5.95	100.35	105.70
1	2A	760	G	N3-C4-C5	5.95	131.57	128.60
1	2A	2734	A	N1-C6-N6	-5.95	115.03	118.60
1	1A	57	C	C2-N1-C1'	-5.95	112.26	118.80
1	1A	312	G	N7-C8-N9	5.95	116.07	113.10
1	1A	435	C	N3-C4-C5	5.95	124.28	121.90
1	1A	2534	A	C2-N3-C4	5.95	113.57	110.60
32	1a	150	C	N3-C4-C5	-5.95	119.52	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	657	G	N3-C2-N2	-5.95	115.74	119.90
1	2A	822	U	N1-C2-N3	5.95	118.47	114.90
1	2A	1934	C	N3-C4-N4	-5.95	113.84	118.00
32	2a	520	A	N1-C6-N6	-5.95	115.03	118.60
1	1A	460	A	N1-C2-N3	5.95	132.27	129.30
1	1A	610	G	C5-N7-C8	5.95	107.27	104.30
32	1a	380	G	C4-C5-N7	-5.95	108.42	110.80
1	2A	524	U	C5-C4-O4	5.95	129.47	125.90
1	1A	769	G	C8-N9-C4	5.94	108.78	106.40
32	1a	1415	G	C6-C5-N7	-5.94	126.83	130.40
1	2A	2133	G	C6-C5-N7	5.94	133.97	130.40
1	2A	2765	A	N1-C6-N6	5.94	122.17	118.60
1	1A	94	C	C6-N1-C2	-5.94	117.92	120.30
1	1A	763	G	N3-C4-N9	-5.94	122.43	126.00
1	1A	1069	A	O4'-C1'-N9	-5.94	103.44	108.20
1	1A	2437	U	C4-C5-C6	5.94	123.27	119.70
32	1a	189(C)	C	C6-N1-C2	-5.94	117.92	120.30
32	1a	718	G	O5'-P-OP2	5.94	117.83	110.70
32	1a	1468	A	C5-C6-N6	-5.94	118.95	123.70
1	2A	1846	G	N1-C6-O6	5.94	123.47	119.90
1	1A	194	G	N7-C8-N9	-5.94	110.13	113.10
1	1A	715	G	C8-N9-C4	5.94	108.78	106.40
32	1a	66	G	C4-C5-N7	5.94	113.18	110.80
1	2A	2009	G	C5-C6-N1	5.94	114.47	111.50
2	2B	51	G	N3-C4-N9	5.94	129.56	126.00
1	1A	2597	G	O5'-P-OP1	5.94	117.83	110.70
1	1A	136	G	N1-C6-O6	5.94	123.46	119.90
1	1A	931	G	C5-N7-C8	5.94	107.27	104.30
1	1A	2514	U	N1-C2-N3	-5.94	111.34	114.90
32	1a	37	U	N3-C2-O2	-5.94	118.04	122.20
1	2A	991	C	OP1-P-OP2	-5.94	110.69	119.60
1	2A	1075	C	C6-N1-C2	-5.94	117.92	120.30
1	2A	1560	G	C5-C6-N1	-5.94	108.53	111.50
1	2A	1826	G	C4-C5-N7	-5.94	108.42	110.80
32	2a	830	G	N1-C6-O6	5.94	123.46	119.90
1	1A	1678	G	C6-N1-C2	-5.94	121.54	125.10
32	1a	435	C	C6-N1-C2	-5.94	117.93	120.30
32	2a	1338	G	N3-C4-C5	-5.94	125.63	128.60
32	2a	1442(B)	A	N1-C6-N6	-5.94	115.04	118.60
1	1A	15	G	N1-C6-O6	5.93	123.46	119.90
1	1A	2203	U	N1-C2-O2	-5.93	118.65	122.80
1	1A	2683	C	N3-C4-C5	-5.93	119.53	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1514	C	N1-C2-O2	5.93	122.46	118.90
1	2A	144	C	C6-N1-C2	-5.93	117.93	120.30
1	2A	1488	G	C8-N9-C4	-5.93	104.03	106.40
1	2A	1501	C	N3-C4-C5	-5.93	119.53	121.90
1	2A	1517	G	C5-C6-N1	-5.93	108.53	111.50
1	2A	1645	G	OP2-P-O3'	5.93	118.26	105.20
1	2A	2451	A	C2-N3-C4	-5.93	107.63	110.60
1	1A	1048	A	C8-N9-C4	-5.93	103.43	105.80
1	1A	1130	U	N3-C2-O2	-5.93	118.05	122.20
1	1A	1236	G	N9-C4-C5	-5.93	103.03	105.40
1	1A	1645	G	C6-N1-C2	-5.93	121.54	125.10
1	1A	2390	U	N3-C4-C5	-5.93	111.04	114.60
1	1A	2778	A	C8-N9-C4	5.93	108.17	105.80
32	1a	254	G	O5'-P-OP2	5.93	117.82	110.70
32	1a	1442	G	C5-C6-O6	-5.93	125.04	128.60
1	2A	423	A	OP1-P-O3'	5.93	118.25	105.20
1	2A	1190	G	OP1-P-O3'	5.93	118.25	105.20
1	2A	2763	G	C5-C6-O6	-5.93	125.04	128.60
1	1A	40	C	C2-N1-C1'	-5.93	112.28	118.80
1	1A	397	G	N1-C6-O6	5.93	123.46	119.90
1	1A	1783	A	OP2-P-O3'	-5.93	92.15	105.20
1	1A	2487	G	C2-N3-C4	-5.93	108.93	111.90
1	2A	94(A)	G	N7-C8-N9	5.93	116.06	113.10
1	1A	231	C	C6-N1-C2	-5.93	117.93	120.30
1	1A	237	C	OP1-P-OP2	5.93	128.49	119.60
1	2A	736	C	N3-C2-O2	5.93	126.05	121.90
1	2A	2462	U	C6-N1-C2	5.93	124.56	121.00
32	2a	346	G	N3-C2-N2	5.93	124.05	119.90
32	2a	380	G	N9-C4-C5	5.93	107.77	105.40
1	1A	804	A	C5-C6-N6	-5.93	118.96	123.70
1	1A	2433	A	C4-C5-C6	5.93	119.96	117.00
1	2A	2012	G	C4-C5-C6	5.93	122.36	118.80
1	2A	2576	G	N3-C4-N9	5.93	129.56	126.00
1	1A	533	G	C5-C6-O6	-5.93	125.04	128.60
1	1A	975(A)	G	N9-C4-C5	5.93	107.77	105.40
1	1A	1132	A	C2-N3-C4	-5.93	107.64	110.60
1	2A	1210	A	N7-C8-N9	5.93	116.76	113.80
32	2a	300	A	N1-C6-N6	5.93	122.16	118.60
1	1A	2060	A	N9-C4-C5	5.92	108.17	105.80
1	1A	2372	G	N7-C8-N9	-5.92	110.14	113.10
29	17	33	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	2A	624	C	O5'-P-OP2	5.92	117.81	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1004	A	O4'-C1'-N9	5.92	112.94	108.20
1	1A	1780	A	O5'-P-OP2	-5.92	100.37	105.70
1	1A	2447	G	C3'-C2'-C1'	-5.92	96.76	101.50
32	1a	1075	C	C6-N1-C2	5.92	122.67	120.30
1	2A	1374	G	N9-C4-C5	-5.92	103.03	105.40
1	1A	193	U	C6-N1-C2	-5.92	117.45	121.00
1	1A	534	U	C4-C5-C6	5.92	123.25	119.70
1	1A	1156	A	O5'-P-OP2	-5.92	100.37	105.70
1	1A	2234	G	N7-C8-N9	-5.92	110.14	113.10
1	1A	2416	C	C6-N1-C2	-5.92	117.93	120.30
1	1A	2424	C	N3-C2-O2	5.92	126.04	121.90
1	1A	2714	G	N7-C8-N9	5.92	116.06	113.10
32	1a	353	A	OP2-P-O3'	5.92	118.22	105.20
1	2A	833	U	C5-C6-N1	5.92	125.66	122.70
1	2A	1471	A	N3-C4-C5	-5.92	122.66	126.80
1	2A	2249	U	N3-C4-O4	-5.92	115.26	119.40
32	2a	1205	U	C6-N1-C2	-5.92	117.45	121.00
1	1A	95	G	OP1-P-OP2	5.92	128.47	119.60
1	1A	371	A	O5'-P-OP2	-5.92	100.37	105.70
1	1A	715	G	C4-N9-C1'	5.92	134.19	126.50
1	1A	1804	C	N3-C4-C5	-5.92	119.53	121.90
1	1A	2705	A	C6-C5-N7	-5.92	128.16	132.30
32	1a	379	C	C6-N1-C2	5.92	122.67	120.30
32	1a	627	G	N1-C6-O6	5.92	123.45	119.90
32	1a	823	G	N9-C4-C5	-5.92	103.03	105.40
1	2A	704	G	N1-C6-O6	-5.92	116.35	119.90
1	2A	2514	U	C5-C6-N1	-5.92	119.74	122.70
1	1A	1019	U	C5-C6-N1	-5.92	119.74	122.70
1	1A	1770	G	C4-C5-N7	-5.92	108.43	110.80
32	2a	729	A	C8-N9-C4	-5.92	103.43	105.80
1	1A	812	C	C2-N3-C4	-5.91	116.94	119.90
1	1A	1169	G	O5'-P-OP1	5.91	117.80	110.70
1	1A	1196	C	N3-C4-C5	5.91	124.27	121.90
1	2A	1032	A	C4-C5-N7	5.91	113.66	110.70
1	2A	2439	A	O5'-P-OP1	5.91	117.80	110.70
1	1A	735	A	N1-C6-N6	5.91	122.15	118.60
1	1A	2392	A	N1-C2-N3	5.91	132.26	129.30
1	1A	2606	C	N1-C2-O2	-5.91	115.35	118.90
1	2A	2513	G	C6-C5-N7	-5.91	126.85	130.40
1	1A	180	G	N3-C2-N2	-5.91	115.76	119.90
1	1A	1888	G	C6-C5-N7	-5.91	126.85	130.40
1	1A	1972	A	C6-C5-N7	-5.91	128.16	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1B	18	G	N1-C6-O6	5.91	123.45	119.90
1	1A	73	A	N1-C2-N3	5.91	132.25	129.30
1	1A	2011	U	N1-C2-O2	-5.91	118.66	122.80
32	1a	1338	G	C4-C5-N7	-5.91	108.44	110.80
1	2A	337	C	O5'-P-OP2	-5.91	100.38	105.70
1	2A	582	G	N1-C6-O6	5.91	123.44	119.90
1	2A	1646	C	C6-N1-C1'	-5.91	113.71	120.80
1	2A	2061	G	C6-C5-N7	-5.91	126.86	130.40
32	2a	244	U	C5-C4-O4	-5.91	122.35	125.90
32	2a	1183	A	OP1-P-O3'	5.91	118.20	105.20
1	1A	2700	C	C6-N1-C2	5.91	122.66	120.30
1	1A	2714	G	C5-N7-C8	-5.91	101.35	104.30
1	1A	1130	U	C4-C5-C6	5.91	123.24	119.70
1	1A	1176	G	OP1-P-O3'	5.91	118.19	105.20
1	1A	1667	G	N3-C2-N2	-5.91	115.77	119.90
32	1a	115	G	P-O3'-C3'	5.91	126.79	119.70
32	1a	153	C	C6-N1-C2	5.91	122.66	120.30
1	2A	31	C	O5'-P-OP1	-5.91	100.39	105.70
1	2A	1553	A	OP2-P-O3'	5.91	118.19	105.20
1	2A	2182	G	C6-C5-N7	5.91	133.94	130.40
32	2a	871	U	N3-C2-O2	-5.91	118.07	122.20
1	1A	143	G	N1-C6-O6	5.90	123.44	119.90
1	1A	725	G	C8-N9-C1'	-5.90	119.32	127.00
1	1A	781	A	C6-N1-C2	-5.90	115.06	118.60
32	1a	58	C	O5'-P-OP1	-5.90	100.39	105.70
32	1a	774	G	C8-N9-C4	-5.90	104.04	106.40
1	2A	374	A	C2-N3-C4	-5.90	107.65	110.60
1	1A	224	G	C4-C5-N7	-5.90	108.44	110.80
1	1A	529	A	N7-C8-N9	5.90	116.75	113.80
1	1A	1786	A	N7-C8-N9	-5.90	110.85	113.80
1	1A	2511	U	C2-N3-C4	-5.90	123.46	127.00
1	2A	29	U	OP2-P-O3'	5.90	118.19	105.20
1	2A	2267	A	C4-N9-C1'	5.90	136.93	126.30
1	1A	844	C	C4-C5-C6	5.90	120.35	117.40
1	1A	1216	G	N3-C4-C5	-5.90	125.65	128.60
1	1A	2767	C	N1-C2-N3	5.90	123.33	119.20
1	2A	808	G	N3-C2-N2	5.90	124.03	119.90
20	2Y	33	LYS	CD-CE-NZ	5.90	125.27	111.70
32	2a	458	C	C6-N1-C2	-5.90	117.94	120.30
1	1A	272(G)	C	O5'-P-OP1	5.90	117.78	110.70
1	1A	784	A	O4'-C1'-N9	5.90	112.92	108.20
1	1A	408	G	OP1-P-O3'	5.90	118.17	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	619	G	N9-C4-C5	-5.90	103.04	105.40
1	1A	627	A	N7-C8-N9	-5.90	110.85	113.80
1	1A	1000	A	N1-C2-N3	-5.90	126.35	129.30
1	1A	2164	C	N3-C4-C5	-5.90	119.54	121.90
1	1A	2619	C	N3-C4-C5	5.90	124.26	121.90
1	2A	2777	G	N3-C4-C5	-5.90	125.65	128.60
1	1A	1758	G	N7-C8-N9	5.90	116.05	113.10
32	2a	23	C	O5'-P-OP2	5.90	117.78	110.70
1	1A	2187	G	N9-C4-C5	-5.89	103.04	105.40
1	2A	154(A)	C	N1-C2-O2	5.89	122.44	118.90
1	2A	1988	C	N3-C2-O2	5.89	126.03	121.90
1	2A	2607	G	OP2-P-O3'	5.89	118.17	105.20
1	1A	72	U	OP1-P-O3'	5.89	118.17	105.20
1	1A	363(B)	G	N9-C4-C5	-5.89	103.04	105.40
1	1A	1634	A	C6-N1-C2	-5.89	115.06	118.60
1	1A	2253	G	O5'-P-OP2	-5.89	100.40	105.70
32	1a	666	G	O5'-P-OP2	-5.89	100.40	105.70
1	2A	999	U	N3-C4-C5	-5.89	111.06	114.60
1	1A	30	G	N1-C2-N3	5.89	127.43	123.90
1	1A	250	G	N7-C8-N9	5.89	116.05	113.10
1	1A	646	A	OP1-P-OP2	-5.89	110.76	119.60
1	1A	838	C	C5-C6-N1	-5.89	118.05	121.00
1	1A	1904	G	C4-C5-N7	-5.89	108.44	110.80
1	1A	2071	A	C4-C5-C6	5.89	119.95	117.00
32	1a	900	A	OP1-P-OP2	-5.89	110.76	119.60
1	2A	1376	C	C5-C6-N1	5.89	123.95	121.00
1	2A	1781	C	O5'-P-OP1	5.89	117.77	110.70
1	1A	32	C	C5-C4-N4	-5.89	116.08	120.20
1	1A	782	A	N1-C6-N6	5.89	122.13	118.60
1	1A	1274	A	C4-C5-N7	5.89	113.64	110.70
1	2A	252	G	C8-N9-C4	5.89	108.76	106.40
1	2A	1853	A	N1-C6-N6	-5.89	115.07	118.60
1	2A	2440	C	C2-N1-C1'	-5.89	112.32	118.80
2	2B	63	G	C8-N9-C4	5.89	108.76	106.40
1	1A	2824	C	OP1-P-OP2	-5.89	110.77	119.60
1	2A	214	G	C5-C6-N1	5.89	114.44	111.50
1	2A	2036	C	N3-C4-N4	-5.89	113.88	118.00
1	1A	496	G	C8-N9-C4	-5.89	104.05	106.40
1	1A	534	U	C2-N1-C1'	-5.89	110.64	117.70
1	1A	586	A	C8-N9-C4	5.89	108.15	105.80
1	1A	1073	A	C2-N3-C4	5.89	113.54	110.60
1	1A	1407	C	N1-C2-O2	-5.89	115.37	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	652(S)	C	C2-N1-C1'	5.89	125.28	118.80
1	2A	1284	A	C5-N7-C8	-5.89	100.96	103.90
1	2A	2371	G	C5-C6-N1	5.89	114.44	111.50
1	2A	2597	G	OP1-P-O3'	5.89	118.15	105.20
32	2a	510	A	N1-C6-N6	-5.89	115.07	118.60
1	2A	1609	A	N1-C6-N6	5.88	122.13	118.60
1	2A	2084	C	C5-C6-N1	-5.88	118.06	121.00
32	1a	379	C	O5'-P-OP2	5.88	117.76	110.70
1	2A	842	G	N1-C2-N2	-5.88	110.91	116.20
1	2A	2886	G	N9-C4-C5	5.88	107.75	105.40
1	1A	328	U	N1-C2-N3	5.88	118.43	114.90
1	1A	736	C	C6-N1-C2	5.88	122.65	120.30
1	1A	785	G	N3-C2-N2	-5.88	115.78	119.90
1	1A	1802	A	N1-C6-N6	5.88	122.13	118.60
1	1A	1964	G	O4'-C1'-N9	-5.88	103.50	108.20
1	1A	2430	A	N1-C6-N6	-5.88	115.07	118.60
1	2A	1283	G	N3-C4-C5	-5.88	125.66	128.60
32	1a	346	G	N3-C2-N2	-5.88	115.78	119.90
1	2A	35	G	OP1-P-OP2	5.88	128.42	119.60
1	2A	371	A	N1-C6-N6	5.88	122.13	118.60
1	1A	458	G	C8-N9-C1'	5.88	134.64	127.00
1	1A	1655	A	N7-C8-N9	-5.88	110.86	113.80
1	1A	1780	A	C6-N1-C2	-5.88	115.07	118.60
1	1A	2083	G	N1-C6-O6	5.88	123.43	119.90
1	1A	231	C	N3-C4-C5	-5.88	119.55	121.90
1	1A	1013	C	N1-C2-O2	-5.88	115.37	118.90
1	1A	2027	G	N3-C4-C5	-5.88	125.66	128.60
32	1a	780	A	C4-C5-N7	5.88	113.64	110.70
1	2A	906	G	O4'-C1'-N9	5.88	112.90	108.20
1	2A	2738	A	C2-N3-C4	-5.88	107.66	110.60
32	1a	1312	G	C8-N9-C4	-5.88	104.05	106.40
1	2A	214	G	N1-C6-O6	-5.88	116.38	119.90
1	2A	1257	C	N3-C4-C5	-5.88	119.55	121.90
1	2A	1900	A	C6-C5-N7	-5.88	128.19	132.30
1	1A	207	A	C6-C5-N7	-5.87	128.19	132.30
1	1A	1901	A	C6-N1-C2	-5.87	115.08	118.60
32	1a	1084	G	C4-N9-C1'	5.87	134.14	126.50
1	2A	1542	A	N9-C4-C5	5.87	108.15	105.80
1	1A	587	C	OP2-P-O3'	5.87	118.12	105.20
1	1A	1301	A	C5-N7-C8	-5.87	100.97	103.90
1	1A	1792	G	N3-C2-N2	-5.87	115.79	119.90
1	1A	2603	G	C5-C6-O6	-5.87	125.08	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2365	G	C8-N9-C4	5.87	108.75	106.40
32	2a	108	G	C4-C5-N7	5.87	113.15	110.80
32	2a	1079	G	C5-C6-O6	5.87	132.12	128.60
32	2a	1370	G	N9-C4-C5	-5.87	103.05	105.40
1	1A	200	U	N1-C2-N3	5.87	118.42	114.90
1	1A	523	C	OP2-P-O3'	5.87	118.11	105.20
1	2A	693	C	N3-C4-C5	5.87	124.25	121.90
1	1A	1041	C	C5-C6-N1	5.87	123.93	121.00
1	1A	1598	C	O5'-P-OP1	-5.87	100.42	105.70
32	1a	105	G	C4-C5-N7	5.87	113.15	110.80
1	2A	1997	G	N3-C4-C5	-5.87	125.67	128.60
32	2a	910	C	C6-N1-C2	5.87	122.65	120.30
1	1A	311	A	O4'-C1'-N9	5.87	112.89	108.20
1	1A	103	A	C8-N9-C1'	-5.87	117.14	127.70
1	1A	260	G	OP1-P-OP2	5.87	128.40	119.60
1	1A	487	C	C6-N1-C2	-5.87	117.95	120.30
1	1A	1344	G	C8-N9-C4	-5.87	104.05	106.40
1	1A	2025	C	C2-N3-C4	5.87	122.83	119.90
1	1A	739	G	C6-C5-N7	-5.86	126.88	130.40
1	1A	1799	G	N3-C4-N9	5.86	129.52	126.00
1	1A	2690	C	N3-C4-N4	5.86	122.11	118.00
1	2A	685	A	N1-C2-N3	-5.86	126.37	129.30
1	2A	1284	A	C4-C5-N7	5.86	113.63	110.70
1	2A	1400	G	N1-C6-O6	5.86	123.42	119.90
32	2a	764	C	N3-C2-O2	-5.86	117.80	121.90
1	1A	969	U	C4-C5-C6	5.86	123.22	119.70
1	1A	1008	C	N1-C2-N3	-5.86	115.10	119.20
1	2A	1883	G	C4-C5-N7	-5.86	108.45	110.80
1	1A	962	G	OP1-P-O3'	5.86	118.09	105.20
32	1a	220	G	C8-N9-C4	-5.86	104.06	106.40
32	1a	557	G	OP1-P-O3'	5.86	118.09	105.20
32	1a	584	G	OP1-P-OP2	5.86	128.39	119.60
32	1a	687	A	C8-N9-C4	-5.86	103.46	105.80
2	2B	103	G	OP2-P-O3'	5.86	118.09	105.20
2	1B	62	C	OP1-P-OP2	5.86	128.39	119.60
1	1A	125	G	N7-C8-N9	-5.86	110.17	113.10
1	1A	413	C	C6-N1-C2	-5.86	117.96	120.30
1	1A	1346	G	C8-N9-C4	5.86	108.74	106.40
1	1A	1553	A	C2-N3-C4	-5.86	107.67	110.60
1	1A	1553	A	C8-N9-C4	5.86	108.14	105.80
1	1A	2576	G	OP2-P-O3'	5.86	118.09	105.20
32	1a	531	U	N3-C2-O2	-5.86	118.10	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1528(A)	A	N1-C6-N6	5.86	122.11	118.60
1	1A	653	A	N1-C6-N6	5.86	122.11	118.60
1	1A	1762	A	C6-C5-N7	5.86	136.40	132.30
1	1A	2033	A	N9-C4-C5	5.86	108.14	105.80
1	1A	2574	G	O5'-P-OP2	5.86	117.73	110.70
32	1a	1376	U	C5-C4-O4	5.86	129.41	125.90
1	2A	1904	G	O5'-P-OP2	-5.86	100.43	105.70
2	2B	61	G	O5'-P-OP1	-5.86	100.43	105.70
2	2B	99	G	N1-C2-N2	5.86	121.47	116.20
1	1A	834	C	C5-C6-N1	-5.85	118.07	121.00
1	1A	947	G	N1-C6-O6	5.85	123.41	119.90
1	1A	1880	C	N3-C4-C5	-5.85	119.56	121.90
32	1a	243	A	N1-C6-N6	-5.85	115.09	118.60
1	2A	245	G	C8-N9-C1'	-5.85	119.39	127.00
14	2S	88	ASP	CB-CG-OD1	5.85	123.57	118.30
1	1A	1099	G	C2-N3-C4	5.85	114.83	111.90
1	1A	1323	U	N3-C4-C5	-5.85	111.09	114.60
1	1A	1553	A	OP2-P-O3'	5.85	118.07	105.20
1	2A	392	C	O5'-P-OP2	5.85	117.72	110.70
1	2A	1600	C	N3-C4-C5	-5.85	119.56	121.90
32	2a	741	G	O5'-P-OP2	-5.85	100.43	105.70
1	1A	1392	A	C5-N7-C8	5.85	106.83	103.90
1	2A	1866	C	N1-C2-O2	5.85	122.41	118.90
1	2A	2478	A	N3-C4-C5	5.85	130.90	126.80
32	2a	1522	U	C4-C5-C6	5.85	123.21	119.70
1	1A	1904	G	C5-N7-C8	5.85	107.22	104.30
1	1A	2394	C	N3-C4-C5	5.85	124.24	121.90
1	1A	2757	A	C8-N9-C4	-5.85	103.46	105.80
1	2A	200	U	C4-C5-C6	5.85	123.21	119.70
1	2A	333	G	N1-C6-O6	5.85	123.41	119.90
1	2A	399	G	N9-C4-C5	-5.85	103.06	105.40
1	2A	1618	A	C5-C6-N6	5.85	128.38	123.70
1	2A	1779	U	O5'-P-OP1	-5.85	100.44	105.70
1	2A	945	A	N1-C6-N6	5.85	122.11	118.60
1	1A	663	G	N1-C2-N2	5.84	121.46	116.20
1	1A	1891	G	C8-N9-C4	5.84	108.74	106.40
1	1A	2586	C	OP1-P-O3'	5.84	118.06	105.20
1	2A	2582	G	OP1-P-O3'	5.84	118.06	105.20
1	1A	2663	G	C5-C6-O6	5.84	132.11	128.60
1	2A	1755	A	N1-C6-N6	-5.84	115.09	118.60
1	2A	1761	C	OP2-P-O3'	5.84	118.05	105.20
1	1A	1312	U	N3-C4-O4	-5.84	115.31	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1779	U	O4'-C1'-N1	5.84	112.87	108.20
1	1A	1954	G	N3-C4-C5	-5.84	125.68	128.60
1	1A	1981	A	C8-N9-C4	-5.84	103.46	105.80
1	1A	2813	A	C8-N9-C4	5.84	108.14	105.80
1	2A	759	G	N3-C2-N2	-5.84	115.81	119.90
1	2A	1796	U	OP1-P-O3'	5.84	118.05	105.20
2	2B	74	U	O5'-P-OP2	-5.84	100.44	105.70
1	1A	2515	C	C4-C5-C6	-5.84	114.48	117.40
2	1B	86	G	C8-N9-C4	5.84	108.74	106.40
1	2A	1314	C	C5-C6-N1	5.84	123.92	121.00
1	2A	2696	U	C4-C5-C6	5.84	123.20	119.70
1	1A	530	G	C4-C5-C6	-5.84	115.30	118.80
1	1A	1459	G	C6-C5-N7	-5.84	126.90	130.40
1	1A	2449	U	C4-C5-C6	5.84	123.20	119.70
1	2A	1384	A	C8-N9-C4	-5.84	103.47	105.80
32	2a	430	A	C5-C6-N6	-5.84	119.03	123.70
1	1A	225	A	O5'-P-OP2	-5.84	100.45	105.70
1	1A	2182	G	N9-C4-C5	5.84	107.73	105.40
1	1A	2514	U	N3-C4-C5	5.84	118.10	114.60
1	2A	2321	G	C4-N9-C1'	5.84	134.09	126.50
15	2T	53	ARG	CB-CA-C	-5.84	98.73	110.40
32	2a	390	C	N3-C4-C5	5.84	124.23	121.90
1	1A	1204	A	N1-C2-N3	5.83	132.22	129.30
1	1A	1578	U	C2-N3-C4	5.83	130.50	127.00
1	1A	1927	A	C5-N7-C8	-5.83	100.98	103.90
1	1A	2354	G	N3-C4-N9	-5.83	122.50	126.00
1	1A	2476	A	C8-N9-C1'	-5.83	117.20	127.70
1	2A	2088	G	N3-C2-N2	-5.83	115.81	119.90
1	1A	776	G	C4-N9-C1'	5.83	134.08	126.50
1	1A	2250	G	OP1-P-OP2	5.83	128.35	119.60
32	1a	889	A	OP1-P-OP2	5.83	128.35	119.60
1	2A	1655	A	N1-C6-N6	5.83	122.10	118.60
12	2Q	79	LEU	CA-CB-CG	-5.83	101.88	115.30
1	1A	1031	G	C4-C5-N7	5.83	113.13	110.80
1	1A	1034	G	C5-C6-N1	5.83	114.42	111.50
1	1A	1683	C	C4-C5-C6	5.83	120.32	117.40
1	1A	2878	U	C6-N1-C2	-5.83	117.50	121.00
1	2A	1040	C	N3-C2-O2	-5.83	117.82	121.90
1	2A	1978	A	C4-C5-C6	5.83	119.92	117.00
1	2A	2791	C	C5-C6-N1	5.83	123.92	121.00
1	1A	843	G	O5'-P-OP2	5.83	117.70	110.70
1	1A	1641	A	C4-C5-C6	5.83	119.92	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	588	U	O5'-P-OP2	-5.83	100.45	105.70
1	1A	725	G	C8-N9-C4	-5.83	104.07	106.40
1	1A	1310	G	OP2-P-O3'	5.83	118.02	105.20
1	1A	2748	A	C5-C6-N6	-5.83	119.04	123.70
1	1A	2760	C	C4-C5-C6	5.83	120.31	117.40
2	2B	1	U	C5-C6-N1	5.83	125.61	122.70
32	2a	1036	G	N3-C4-N9	5.83	129.50	126.00
32	2a	1137	C	C6-N1-C1'	5.83	127.79	120.80
1	1A	885	C	C5-C6-N1	5.83	123.91	121.00
1	1A	2659	G	C2-N3-C4	-5.83	108.99	111.90
1	1A	569	U	O5'-P-OP1	-5.83	100.46	105.70
1	1A	2502	G	C8-N9-C4	-5.83	104.07	106.40
1	1A	2508	G	C5-C6-N1	5.83	114.41	111.50
32	1a	1338	G	C5-C6-O6	5.83	132.10	128.60
1	2A	1702	G	C5-C6-N1	5.83	114.41	111.50
32	2a	972	C	C6-N1-C2	-5.83	117.97	120.30
1	1A	1812	A	C8-N9-C4	-5.82	103.47	105.80
1	1A	1989	G	N9-C4-C5	-5.82	103.07	105.40
1	1A	2730	C	OP2-P-O3'	5.82	118.01	105.20
2	1B	57	A	OP2-P-O3'	5.82	118.01	105.20
1	2A	1940	U	C6-N1-C2	-5.82	117.51	121.00
2	2B	116	G	OP1-P-OP2	5.82	128.33	119.60
32	2a	533	A	C5-C6-N6	-5.82	119.04	123.70
1	1A	491	G	N3-C2-N2	-5.82	115.83	119.90
1	1A	989	G	C5-C6-O6	-5.82	125.11	128.60
1	1A	1762	A	C4-C5-N7	-5.82	107.79	110.70
1	1A	2041	U	N1-C2-N3	5.82	118.39	114.90
1	1A	2166	G	C5-C6-N1	-5.82	108.59	111.50
1	1A	2770	G	N3-C4-N9	5.82	129.49	126.00
1	2A	1776	G	C4-N9-C1'	5.82	134.07	126.50
1	2A	2031	A	C6-N1-C2	-5.82	115.11	118.60
1	1A	867	C	N3-C4-C5	-5.82	119.57	121.90
1	1A	1710	C	OP2-P-O3'	5.82	118.00	105.20
1	2A	2818	G	N1-C6-O6	-5.82	116.41	119.90
4	2E	149	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	1A	477	A	OP1-P-OP2	5.82	128.33	119.60
1	1A	505	A	C8-N9-C4	-5.82	103.47	105.80
2	1B	31	C	N1-C2-O2	5.82	122.39	118.90
1	2A	177	G	O4'-C1'-N9	5.82	112.85	108.20
1	2A	446	G	N3-C4-C5	5.82	131.51	128.60
1	2A	786	C	C6-N1-C2	5.82	122.63	120.30
1	2A	1580	A	N1-C6-N6	5.82	122.09	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1772	G	N9-C1'-C2'	-5.82	105.60	112.00
2	2B	89	G	O5'-P-OP2	-5.82	100.47	105.70
1	1A	151	C	C6-N1-C2	5.82	122.63	120.30
1	1A	1598	C	OP2-P-O3'	5.82	117.99	105.20
32	1a	343	U	O4'-C1'-N1	5.82	112.85	108.20
32	1a	380	G	N9-C4-C5	5.82	107.73	105.40
1	2A	203	C	C5-C4-N4	-5.82	116.13	120.20
1	2A	1415	U	N3-C4-O4	-5.82	115.33	119.40
1	2A	1891	G	N3-C4-C5	5.82	131.51	128.60
1	2A	2804	C	N3-C4-C5	-5.82	119.57	121.90
32	2a	1301	U	C5-C6-N1	-5.82	119.79	122.70
1	1A	819	A	OP2-P-O3'	5.81	117.99	105.20
1	2A	570	G	C5-C6-N1	5.81	114.41	111.50
1	2A	1400	G	N7-C8-N9	5.81	116.01	113.10
1	2A	1494	A	N1-C2-N3	5.81	132.21	129.30
1	2A	2296	U	N1-C2-O2	5.81	126.87	122.80
32	2a	1096	C	C6-N1-C2	-5.81	117.97	120.30
1	1A	2426	A	C8-N9-C4	-5.81	103.47	105.80
1	2A	408	G	O5'-P-OP2	-5.81	100.47	105.70
32	2a	533	A	C6-N1-C2	-5.81	115.11	118.60
32	2a	1259	C	C6-N1-C2	-5.81	117.97	120.30
1	1A	1476	C	N3-C4-C5	-5.81	119.58	121.90
1	2A	18	C	O5'-P-OP1	-5.81	100.47	105.70
1	2A	2579	C	N3-C4-C5	5.81	124.22	121.90
1	1A	361	G	N3-C4-C5	5.81	131.50	128.60
1	1A	1900	A	C8-N9-C4	-5.81	103.48	105.80
32	1a	199	G	C8-N9-C4	5.81	108.72	106.40
32	1a	1016	A	N9-C4-C5	-5.81	103.48	105.80
32	1a	1387	G	N1-C6-O6	-5.81	116.42	119.90
1	2A	738	G	C6-C5-N7	5.81	133.89	130.40
1	1A	1824	G	C4-C5-N7	5.81	113.12	110.80
2	1B	99	G	N1-C6-O6	5.81	123.38	119.90
1	2A	1952	A	O5'-P-OP1	-5.81	100.47	105.70
1	2A	2206	G	N3-C4-C5	5.81	131.50	128.60
1	1A	2413	G	O5'-P-OP1	5.81	117.67	110.70
1	1A	2679	A	C5-C6-N1	5.81	120.60	117.70
32	1a	710	G	C6-C5-N7	-5.81	126.92	130.40
1	2A	1642	G	OP1-P-OP2	5.81	128.31	119.60
1	1A	805	G	C8-N9-C4	-5.80	104.08	106.40
1	1A	1082	U	C6-N1-C2	-5.80	117.52	121.00
1	1A	2729	G	N3-C4-C5	5.80	131.50	128.60
1	2A	462	C	C6-N1-C2	5.80	122.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1426	G	C4-C5-N7	-5.80	108.48	110.80
1	2A	2446	G	N1-C2-N3	5.80	127.38	123.90
1	1A	1158	C	N1-C2-N3	5.80	123.26	119.20
32	1a	244	U	O5'-P-OP2	-5.80	100.48	105.70
1	2A	331	A	N9-C4-C5	5.80	108.12	105.80
1	2A	645	C	C2-N3-C4	5.80	122.80	119.90
32	2a	5	U	C6-N1-C2	-5.80	117.52	121.00
32	2a	1027	C	C2-N1-C1'	5.80	125.18	118.80
1	1A	805	G	C5-N7-C8	-5.80	101.40	104.30
1	1A	1745(A)	C	C6-N1-C2	-5.80	117.98	120.30
1	2A	858	U	N3-C2-O2	-5.80	118.14	122.20
1	2A	1512	U	N3-C4-C5	-5.80	111.12	114.60
1	2A	2478	A	N9-C4-C5	-5.80	103.48	105.80
1	2A	2766	G	N3-C2-N2	-5.80	115.84	119.90
1	1A	128	C	C5-C6-N1	-5.80	118.10	121.00
1	1A	2083	G	C2-N3-C4	-5.80	109.00	111.90
1	1A	2253	G	C2-N3-C4	-5.80	109.00	111.90
1	2A	659	C	C2-N1-C1'	-5.80	112.42	118.80
1	2A	1381	G	N9-C4-C5	5.80	107.72	105.40
1	2A	2606	C	C2-N3-C4	5.80	122.80	119.90
32	2a	1037	C	C5-C6-N1	5.80	123.90	121.00
1	1A	1516	C	C6-N1-C2	-5.80	117.98	120.30
1	1A	1661	G	O5'-P-OP1	5.80	117.66	110.70
1	1A	2321	G	OP2-P-O3'	5.80	117.96	105.20
1	1A	2881	C	OP1-P-O3'	5.80	117.96	105.20
1	2A	187	G	C4-C5-N7	5.80	113.12	110.80
1	2A	618	C	C6-N1-C2	5.80	122.62	120.30
1	2A	659	C	O5'-P-OP1	5.80	117.66	110.70
1	2A	1990	C	N1-C2-N3	5.80	123.26	119.20
1	1A	2050	C	N3-C2-O2	5.80	125.96	121.90
1	1A	2359	C	C6-N1-C2	5.80	122.62	120.30
1	2A	493	G	N1-C6-O6	5.80	123.38	119.90
1	2A	1899	G	C5-C6-O6	-5.80	125.12	128.60
1	1A	729	G	N3-C2-N2	-5.79	115.84	119.90
1	2A	2133	G	C8-N9-C1'	5.79	134.53	127.00
32	2a	769	G	OP2-P-O3'	5.79	117.95	105.20
1	1A	175	G	N1-C2-N2	-5.79	110.99	116.20
1	1A	1812	A	C2-N3-C4	5.79	113.50	110.60
32	1a	1467	G	N1-C6-O6	-5.79	116.42	119.90
1	2A	218	A	C2-N3-C4	-5.79	107.70	110.60
1	2A	1309	G	OP2-P-O3'	5.79	117.95	105.20
1	2A	2249	U	C5-C4-O4	5.79	129.38	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1176	A	C8-N9-C4	-5.79	103.48	105.80
1	1A	1784	A	N1-C6-N6	-5.79	115.12	118.60
1	2A	948	G	N3-C2-N2	-5.79	115.85	119.90
1	2A	2659	G	O5'-P-OP2	-5.79	100.49	105.70
1	1A	376	C	N3-C4-N4	-5.79	113.95	118.00
32	1a	312	C	OP2-P-O3'	5.79	117.94	105.20
1	1A	576	U	OP1-P-OP2	5.79	128.28	119.60
1	1A	2584	U	C5-C6-N1	5.79	125.59	122.70
1	1A	2615	U	N3-C4-C5	5.79	118.07	114.60
1	2A	246	C	C5-C6-N1	-5.79	118.11	121.00
1	2A	1818	U	C5-C6-N1	-5.79	119.81	122.70
32	2a	728	A	C8-N9-C4	-5.79	103.48	105.80
1	1A	271(X)	G	C8-N9-C4	-5.79	104.08	106.40
1	1A	667	U	N3-C2-O2	5.79	126.25	122.20
32	1a	863	U	C6-N1-C1'	5.79	129.30	121.20
1	2A	219	G	C6-N1-C2	-5.79	121.63	125.10
1	2A	915	C	N1-C2-O2	5.79	122.37	118.90
32	2a	122	G	N3-C4-C5	-5.79	125.71	128.60
1	1A	1212	G	C5-N7-C8	5.79	107.19	104.30
1	1A	1849	G	N3-C4-N9	-5.79	122.53	126.00
1	1A	2879	C	O5'-P-OP1	-5.79	100.49	105.70
1	2A	415	A	O5'-P-OP2	-5.79	100.49	105.70
1	2A	1970	A	C8-N9-C4	-5.79	103.49	105.80
1	2A	2576	G	C5-C6-N1	5.79	114.39	111.50
32	2a	1531	A	N1-C6-N6	5.79	122.07	118.60
1	1A	1320	C	C2-N3-C4	-5.78	117.01	119.90
32	1a	738	C	N3-C4-C5	-5.78	119.59	121.90
32	2a	391	G	C4-C5-N7	5.78	113.11	110.80
32	2a	1274	G	C8-N9-C4	-5.78	104.09	106.40
1	1A	126	A	O5'-P-OP1	-5.78	100.50	105.70
1	1A	139(A)	G	N9-C4-C5	-5.78	103.09	105.40
1	1A	226	G	N1-C2-N3	-5.78	120.43	123.90
1	1A	707	G	C5-C6-O6	-5.78	125.13	128.60
1	1A	1505	C	C6-N1-C2	-5.78	117.99	120.30
1	2A	839	U	C2-N1-C1'	-5.78	110.76	117.70
1	1A	391	G	C4-N9-C1'	5.78	134.01	126.50
1	1A	985	C	N1-C2-O2	5.78	122.37	118.90
1	1A	1216	G	C4-C5-C6	5.78	122.27	118.80
1	1A	2576	G	OP1-P-OP2	-5.78	110.93	119.60
1	1A	2853	C	C6-N1-C2	5.78	122.61	120.30
1	2A	1777	U	N3-C2-O2	-5.78	118.15	122.20
32	2a	894	G	N1-C6-O6	5.78	123.37	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2444	G	N1-C6-O6	-5.78	116.43	119.90
1	2A	1312	U	N3-C4-C5	-5.78	111.13	114.60
1	2A	2489	G	OP2-P-O3'	5.78	117.91	105.20
32	2a	1026	G	N3-C4-C5	-5.78	125.71	128.60
1	1A	333	G	OP2-P-O3'	5.78	117.91	105.20
1	1A	1564	C	C4-C5-C6	5.78	120.29	117.40
1	1A	2548	G	C4-C5-N7	-5.78	108.49	110.80
32	1a	297	G	C2-N3-C4	-5.78	109.01	111.90
32	1a	1442	G	C4-N9-C1'	5.78	134.01	126.50
1	2A	2504	U	O5'-P-OP2	-5.78	100.50	105.70
2	2B	102	A	C8-N9-C4	5.78	108.11	105.80
32	2a	121	C	C5-C4-N4	-5.78	116.16	120.20
1	1A	1175	U	OP1-P-O3'	5.78	117.90	105.20
1	1A	1301	A	N7-C8-N9	5.78	116.69	113.80
1	1A	2117	A	C5-C6-N1	5.78	120.59	117.70
13	1R	67	LEU	CA-CB-CG	5.78	128.59	115.30
16	1U	20	LEU	CB-CG-CD2	-5.78	101.18	111.00
1	2A	139(A)	G	N7-C8-N9	-5.78	110.21	113.10
1	2A	1797	C	C5-C6-N1	-5.78	118.11	121.00
1	2A	2808	U	C6-N1-C2	5.78	124.47	121.00
32	2a	1148	U	N1-C2-N3	5.78	118.36	114.90
32	2a	1156	G	C8-N9-C4	-5.78	104.09	106.40
32	2a	1189	C	N1-C2-O2	5.78	122.36	118.90
1	1A	725	G	C4-C5-C6	5.77	122.26	118.80
1	1A	1815	A	C6-N1-C2	-5.77	115.14	118.60
1	1A	2572	A	C4-C5-C6	5.77	119.89	117.00
32	1a	702	A	O5'-P-OP2	-5.77	100.50	105.70
1	2A	2735	G	C6-C5-N7	5.77	133.86	130.40
1	2A	2794	C	C5-C6-N1	5.77	123.89	121.00
1	1A	767	U	N3-C4-C5	-5.77	111.14	114.60
1	1A	2002	G	C8-N9-C4	5.77	108.71	106.40
1	1A	2745	C	C6-N1-C2	-5.77	117.99	120.30
16	1U	19	LYS	CD-CE-NZ	-5.77	98.42	111.70
1	2A	1385	G	O4'-C1'-N9	5.77	112.82	108.20
1	2A	2390	U	C6-N1-C2	-5.77	117.54	121.00
1	2A	2453	A	N9-C4-C5	-5.77	103.49	105.80
1	1A	185	U	N1-C2-O2	-5.77	118.76	122.80
1	1A	2422	A	C2-N3-C4	-5.77	107.72	110.60
1	2A	1970	A	N9-C4-C5	5.77	108.11	105.80
2	2B	24	G	N9-C4-C5	-5.77	103.09	105.40
32	2a	1465	C	C2-N1-C1'	5.77	125.15	118.80
1	1A	434	U	O5'-P-OP2	-5.77	100.51	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1085	A	C8-N9-C4	-5.77	103.49	105.80
1	1A	1787	A	C5-N7-C8	-5.77	101.02	103.90
32	2a	820	U	N3-C2-O2	-5.77	118.16	122.20
32	2a	1065	U	P-O3'-C3'	5.77	126.62	119.70
1	1A	1614	A	N7-C8-N9	-5.77	110.92	113.80
1	1A	2286	A	N1-C2-N3	5.77	132.18	129.30
3	1D	3	VAL	N-CA-C	-5.77	95.42	111.00
32	1a	533	A	C6-N1-C2	-5.77	115.14	118.60
32	1a	570	G	C4-C5-N7	5.77	113.11	110.80
32	1a	715	A	C2-N3-C4	-5.77	107.72	110.60
1	2A	800	A	N7-C8-N9	5.77	116.68	113.80
1	2A	925	C	N3-C4-N4	-5.77	113.96	118.00
1	1A	1045	A	O4'-C1'-N9	5.76	112.81	108.20
1	1A	1954	G	N3-C4-N9	5.76	129.46	126.00
1	1A	2690	C	OP1-P-O3'	5.76	117.88	105.20
32	1a	1486	G	C5-C6-N1	-5.76	108.62	111.50
1	2A	465	G	C5-C6-O6	-5.76	125.14	128.60
2	2B	74	U	N3-C2-O2	-5.76	118.17	122.20
32	2a	889	A	OP1-P-OP2	5.76	128.25	119.60
1	1A	1721	G	N7-C8-N9	5.76	115.98	113.10
32	1a	823	G	N3-C4-C5	5.76	131.48	128.60
1	2A	2311	A	N1-C6-N6	-5.76	115.14	118.60
32	2a	226	G	C4-N9-C1'	-5.76	119.01	126.50
32	2a	759	A	C8-N9-C4	5.76	108.11	105.80
1	1A	696	G	N3-C2-N2	-5.76	115.87	119.90
1	1A	783	A	C5-C6-N6	5.76	128.31	123.70
32	1a	1031	G	C8-N9-C4	-5.76	104.10	106.40
1	1A	647	G	O5'-P-OP1	-5.76	100.52	105.70
1	1A	1695	G	C4-C5-C6	5.76	122.26	118.80
1	1A	2451	A	N9-C4-C5	5.76	108.10	105.80
1	2A	2274	A	N1-C6-N6	-5.76	115.14	118.60
1	1A	636	G	N1-C6-O6	5.76	123.36	119.90
1	1A	912	C	C5-C6-N1	5.76	123.88	121.00
1	1A	2600	A	C2-N3-C4	5.76	113.48	110.60
1	1A	2631	G	O5'-P-OP1	-5.76	100.52	105.70
1	2A	1798	U	N3-C2-O2	-5.76	118.17	122.20
1	2A	2724	C	N3-C4-N4	-5.76	113.97	118.00
1	1A	979	G	N3-C2-N2	-5.76	115.87	119.90
1	1A	1609	A	O5'-P-OP1	-5.76	100.52	105.70
1	1A	2517	C	N1-C2-N3	-5.76	115.17	119.20
1	1A	2542	A	N9-C4-C5	5.76	108.10	105.80
32	1a	970	C	N1-C2-O2	5.76	122.35	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	843	G	C8-N9-C4	5.76	108.70	106.40
1	2A	1637	A	OP1-P-OP2	-5.76	110.97	119.60
1	2A	2502	G	N7-C8-N9	5.76	115.98	113.10
32	2a	299	G	C8-N9-C4	5.76	108.70	106.40
32	2a	748	C	N3-C2-O2	5.76	125.93	121.90
1	1A	934	G	C5-N7-C8	5.75	107.18	104.30
1	1A	2711	A	O5'-P-OP1	-5.75	100.52	105.70
32	1a	623	C	C5-C6-N1	5.75	123.88	121.00
1	2A	999	U	OP1-P-O3'	5.75	117.86	105.20
1	1A	1060	U	C5-C4-O4	-5.75	122.45	125.90
1	1A	1439	A	C8-N9-C4	5.75	108.10	105.80
1	1A	1756	G	N1-C6-O6	-5.75	116.45	119.90
1	1A	2259	G	N9-C4-C5	-5.75	103.10	105.40
1	1A	2808	U	N3-C4-O4	5.75	123.43	119.40
32	1a	616	G	C8-N9-C4	-5.75	104.10	106.40
1	2A	2511	U	C6-N1-C2	-5.75	117.55	121.00
1	2A	2573	C	C2-N1-C1'	5.75	125.13	118.80
32	2a	1528	U	OP1-P-OP2	5.75	128.23	119.60
1	1A	154(A)	C	N1-C2-N3	-5.75	115.17	119.20
1	1A	582	G	N1-C2-N3	5.75	127.35	123.90
1	1A	1637	A	OP1-P-OP2	-5.75	110.97	119.60
1	1A	2003	G	N9-C4-C5	-5.75	103.10	105.40
32	1a	1495	U	N3-C4-C5	-5.75	111.15	114.60
1	2A	2313	C	N3-C4-C5	-5.75	119.60	121.90
1	2A	2667	C	N3-C4-C5	-5.75	119.60	121.90
32	2a	254	G	O5'-P-OP1	-5.75	100.52	105.70
32	2a	901	A	C6-C5-N7	-5.75	128.27	132.30
32	2a	1530	G	O5'-P-OP1	5.75	117.60	110.70
1	1A	1648	C	O5'-P-OP2	5.75	117.60	110.70
32	1a	521	G	C5-C6-N1	5.75	114.38	111.50
1	2A	484	C	O5'-P-OP2	-5.75	100.53	105.70
1	1A	1256	G	C8-N9-C1'	-5.75	119.53	127.00
1	1A	1659	U	OP1-P-OP2	5.75	128.22	119.60
1	1A	1694	C	N1-C2-O2	-5.75	115.45	118.90
1	1A	2062	A	N1-C2-N3	5.75	132.18	129.30
1	1A	2247	A	C5-C6-N1	-5.75	114.83	117.70
32	1a	1053	G	C8-N9-C4	5.75	108.70	106.40
1	2A	1567	A	OP1-P-O3'	5.75	117.84	105.20
32	2a	24	U	N1-C2-O2	-5.75	118.78	122.80
1	1A	1208	C	C2-N3-C4	-5.75	117.03	119.90
1	1A	2252	G	N3-C2-N2	5.75	123.92	119.90
1	1A	2447	G	OP1-P-OP2	-5.75	110.98	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1R	81	ASP	CB-CG-OD1	5.75	123.47	118.30
1	2A	1200	C	C4-C5-C6	5.75	120.27	117.40
1	2A	1782	C	C4-C5-C6	5.75	120.27	117.40
1	2A	2378	A	C4-N9-C1'	5.75	136.65	126.30
1	2A	2531	A	C8-N9-C4	5.75	108.10	105.80
1	1A	1209	G	C4-C5-N7	5.75	113.10	110.80
1	1A	2206	G	C8-N9-C1'	5.75	134.47	127.00
1	2A	800	A	C8-N9-C4	-5.75	103.50	105.80
1	2A	2679	A	N7-C8-N9	-5.75	110.93	113.80
32	2a	697	U	C6-N1-C2	5.75	124.45	121.00
32	2a	926	G	N1-C2-N2	-5.75	111.03	116.20
32	2a	1506	U	C5-C4-O4	-5.75	122.45	125.90
1	1A	686	G	C5-N7-C8	-5.74	101.43	104.30
1	1A	2499	C	O5'-P-OP1	5.74	117.59	110.70
1	2A	1840	G	C2-N3-C4	5.74	114.77	111.90
1	1A	582	G	C8-N9-C4	5.74	108.70	106.40
1	1A	2386	C	N3-C2-O2	-5.74	117.88	121.90
32	1a	823	G	O5'-P-OP2	5.74	117.59	110.70
1	2A	1286	A	C5-C6-N6	5.74	128.29	123.70
32	2a	1294	G	C4-N9-C1'	-5.74	119.04	126.50
1	1A	831	G	OP2-P-O3'	-5.74	92.57	105.20
1	1A	1163	G	N9-C4-C5	-5.74	103.10	105.40
1	1A	2616	C	OP2-P-O3'	5.74	117.83	105.20
1	1A	2781	A	O4'-C1'-N9	-5.74	103.61	108.20
2	1B	50	G	N1-C6-O6	-5.74	116.46	119.90
32	1a	1529	G	N9-C4-C5	5.74	107.70	105.40
1	2A	144	C	N3-C4-C5	-5.74	119.60	121.90
1	2A	1047	G	C8-N9-C4	-5.74	104.10	106.40
1	2A	2093	G	C8-N9-C4	5.74	108.70	106.40
1	2A	2596	U	N1-C2-O2	-5.74	118.78	122.80
32	2a	1442	G	C6-C5-N7	-5.74	126.95	130.40
1	1A	780	G	N3-C2-N2	-5.74	115.88	119.90
1	1A	933	A	N1-C2-N3	5.74	132.17	129.30
2	1B	86	G	N1-C6-O6	5.74	123.34	119.90
32	1a	168	G	N3-C2-N2	5.74	123.92	119.90
32	1a	422	C	N3-C2-O2	-5.74	117.88	121.90
1	2A	451	C	C2-N3-C4	-5.74	117.03	119.90
1	2A	683	C	O5'-P-OP1	-5.74	100.54	105.70
1	2A	767	U	N3-C2-O2	-5.74	118.18	122.20
1	2A	2579	C	C6-N1-C2	5.74	122.59	120.30
2	2B	59	A	O5'-P-OP2	-5.74	100.53	105.70
32	2a	357	G	N9-C4-C5	5.74	107.69	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	251	A	C2-N3-C4	5.74	113.47	110.60
32	2a	714	G	N1-C6-O6	5.74	123.34	119.90
1	1A	686	G	C5-C6-N1	5.74	114.37	111.50
1	1A	1219	G	N3-C4-C5	5.74	131.47	128.60
1	1A	1984	G	C2-N3-C4	5.74	114.77	111.90
1	1A	2037	G	C8-N9-C4	5.74	108.69	106.40
32	1a	841	U	N1-C2-O2	5.74	126.81	122.80
32	1a	1502	A	O5'-P-OP1	5.74	117.58	110.70
1	2A	784	A	C8-N9-C1'	5.74	138.02	127.70
1	2A	1031	G	N9-C4-C5	-5.74	103.11	105.40
1	2A	1337	G	OP1-P-O3'	5.74	117.82	105.20
1	2A	1640	C	N1-C2-O2	5.74	122.34	118.90
32	2a	1206	G	N3-C4-N9	5.74	129.44	126.00
1	1A	528	A	O4'-C1'-N9	-5.73	103.61	108.20
1	1A	2534	A	C6-N1-C2	-5.73	115.16	118.60
1	1A	1227	G	N1-C2-N3	5.73	127.34	123.90
1	1A	1753	G	N7-C8-N9	5.73	115.97	113.10
1	1A	2063	C	C6-N1-C2	5.73	122.59	120.30
1	1A	2283	C	O5'-P-OP1	5.73	117.58	110.70
1	1A	2663	G	O5'-P-OP1	-5.73	100.54	105.70
2	1B	51	G	C6-C5-N7	-5.73	126.96	130.40
32	1a	858	G	N1-C6-O6	-5.73	116.46	119.90
32	1a	1447	A	C8-N9-C4	-5.73	103.51	105.80
1	2A	858	U	C6-N1-C2	-5.73	117.56	121.00
1	2A	2460	U	C5-C6-N1	-5.73	119.83	122.70
32	2a	857	C	C6-N1-C2	5.73	122.59	120.30
1	1A	330	A	N7-C8-N9	5.73	116.67	113.80
1	1A	640	C	N1-C2-O2	-5.73	115.46	118.90
1	1A	1028	A	N7-C8-N9	-5.73	110.93	113.80
1	1A	1520	G	C5-C6-O6	5.73	132.04	128.60
32	1a	1435	G	N3-C2-N2	-5.73	115.89	119.90
32	1a	1466	C	O4'-C1'-N1	5.73	112.78	108.20
1	2A	738	G	OP1-P-O3'	5.73	117.81	105.20
1	2A	966	G	N3-C4-C5	-5.73	125.73	128.60
1	2A	1364	G	N7-C8-N9	-5.73	110.23	113.10
1	2A	675	A	OP1-P-O3'	-5.73	92.60	105.20
1	2A	2023	G	C5-C6-N1	5.73	114.36	111.50
1	1A	1864	U	N3-C4-C5	-5.73	111.16	114.60
1	1A	2004	G	N3-C4-C5	5.73	131.46	128.60
1	1A	2009	G	N1-C2-N2	5.73	121.36	116.20
1	2A	774	A	C5-C6-N1	-5.73	114.84	117.70
1	2A	859	G	C5-C6-N1	-5.73	108.64	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	945	A	C2-N3-C4	-5.73	107.74	110.60
1	2A	1262	A	C5-N7-C8	-5.73	101.04	103.90
1	2A	1542	A	N1-C6-N6	-5.73	115.16	118.60
1	2A	2032	G	OP1-P-O3'	5.73	117.80	105.20
32	2a	7	G	C4-N9-C1'	-5.73	119.05	126.50
1	1A	1692	U	C4-C5-C6	5.73	123.14	119.70
32	1a	259	G	C4-C5-N7	5.73	113.09	110.80
1	2A	1601	G	OP1-P-O3'	5.73	117.80	105.20
1	1A	2363	C	O5'-P-OP1	5.72	117.57	110.70
1	1A	2763	G	C8-N9-C4	5.72	108.69	106.40
32	1a	421	U	N3-C2-O2	-5.72	118.19	122.20
32	1a	1028	C	C5-C6-N1	5.72	123.86	121.00
1	2A	509	C	N3-C2-O2	-5.72	117.89	121.90
1	2A	2407	G	N1-C2-N2	-5.72	111.05	116.20
32	2a	1294	G	N3-C4-N9	-5.72	122.57	126.00
1	1A	705	A	O5'-P-OP2	-5.72	100.55	105.70
1	1A	995	C	N1-C2-O2	5.72	122.33	118.90
1	1A	1031	G	C5-C6-O6	-5.72	125.17	128.60
1	1A	1082	U	N3-C2-O2	-5.72	118.19	122.20
1	2A	569	U	N3-C2-O2	5.72	126.20	122.20
1	2A	1328	G	C5-C6-O6	-5.72	125.17	128.60
1	2A	2235	G	OP2-P-O3'	5.72	117.79	105.20
1	1A	596	G	O5'-P-OP1	-5.72	100.55	105.70
1	1A	1328	G	N1-C2-N3	5.72	127.33	123.90
1	2A	42	G	O5'-P-OP1	-5.72	100.55	105.70
1	2A	2049	G	C5-C6-O6	5.72	132.03	128.60
1	1A	31	C	OP1-P-OP2	5.72	128.18	119.60
1	1A	755	C	N3-C4-N4	5.72	122.00	118.00
1	1A	2028	U	C5-C4-O4	5.72	129.33	125.90
1	1A	2561	A	C4-C5-N7	-5.72	107.84	110.70
1	2A	1992	G	N9-C4-C5	-5.72	103.11	105.40
1	2A	2337	G	C5-C6-O6	5.72	132.03	128.60
1	1A	513	A	OP2-P-O3'	5.72	117.77	105.20
1	1A	908	C	OP2-P-O3'	5.72	117.78	105.20
1	1A	1427	A	N1-C6-N6	-5.72	115.17	118.60
1	1A	1854	A	N1-C6-N6	5.72	122.03	118.60
1	1A	1900	A	C6-N1-C2	-5.72	115.17	118.60
1	1A	2056	G	C6-C5-N7	-5.72	126.97	130.40
1	1A	2585	U	OP1-P-O3'	5.72	117.78	105.20
1	1A	2847	U	C2-N1-C1'	-5.72	110.84	117.70
32	1a	292	G	C8-N9-C4	5.72	108.69	106.40
32	1a	522	C	C6-N1-C2	5.72	122.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	660	G	C4-C5-N7	5.72	113.09	110.80
32	1a	899	C	C6-N1-C2	5.72	122.59	120.30
1	2A	399	G	N1-C6-O6	5.72	123.33	119.90
1	2A	453	C	N3-C4-N4	-5.72	114.00	118.00
1	2A	1395	A	O4'-C1'-N9	5.72	112.77	108.20
1	1A	569	U	C6-N1-C2	5.71	124.43	121.00
1	1A	988	A	C5-C6-N6	-5.71	119.13	123.70
1	1A	1427	A	C5-N7-C8	5.71	106.76	103.90
1	1A	1609	A	C5-C6-N6	-5.71	119.13	123.70
1	1A	1943	U	C2-N3-C4	-5.71	123.57	127.00
1	2A	710	G	C2-N3-C4	-5.71	109.04	111.90
1	2A	1022	G	C8-N9-C4	-5.71	104.11	106.40
1	2A	1589	C	N1-C2-O2	5.71	122.33	118.90
1	2A	2065	C	N3-C4-N4	-5.71	114.00	118.00
1	2A	2711	A	C8-N9-C4	5.71	108.09	105.80
32	2a	342	C	C5-C6-N1	5.71	123.86	121.00
32	2a	1126	U	C5-C6-N1	5.71	125.56	122.70
1	1A	1309	G	C6-C5-N7	-5.71	126.97	130.40
32	1a	229	U	N3-C4-O4	5.71	123.40	119.40
1	2A	391	G	C6-N1-C2	-5.71	121.67	125.10
32	2a	508	C	N1-C2-O2	5.71	122.33	118.90
1	1A	1062	G	N3-C4-N9	5.71	129.43	126.00
1	1A	2599	G	N3-C4-N9	-5.71	122.57	126.00
32	1a	572	A	C4-C5-C6	-5.71	114.14	117.00
32	1a	1138	G	C2-N3-C4	5.71	114.76	111.90
1	2A	1274	A	C5-C6-N6	-5.71	119.13	123.70
1	2A	1381	G	C5-C6-O6	5.71	132.03	128.60
32	2a	970	C	N1-C2-O2	5.71	122.33	118.90
1	1A	2582	G	N1-C2-N2	-5.71	111.06	116.20
1	1A	408	G	N3-C4-C5	-5.71	125.75	128.60
1	1A	469	G	C8-N9-C4	-5.71	104.12	106.40
1	1A	1267	U	OP1-P-O3'	5.71	117.76	105.20
1	1A	1327	C	C4-C5-C6	5.71	120.25	117.40
1	1A	2443	C	N1-C2-O2	-5.71	115.47	118.90
32	2a	525	C	C4-C5-C6	-5.71	114.55	117.40
1	1A	254	G	N1-C6-O6	5.71	123.32	119.90
1	1A	347	A	C5-C6-N1	-5.71	114.85	117.70
1	1A	939	G	N9-C4-C5	5.71	107.68	105.40
1	1A	1308	A	N9-C4-C5	5.71	108.08	105.80
1	1A	2564	A	C4-C5-C6	5.71	119.85	117.00
1	1A	2820	A	N1-C2-N3	5.71	132.15	129.30
32	1a	543	C	O5'-P-OP1	-5.71	100.56	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	780	A	C5-N7-C8	-5.71	101.05	103.90
1	2A	1663	C	C2-N3-C4	-5.71	117.05	119.90
1	1A	536	A	C4-C5-N7	5.71	113.55	110.70
1	2A	1996	C	C6-N1-C2	5.71	122.58	120.30
1	1A	614(A)	U	C2-N1-C1'	5.70	124.54	117.70
1	1A	1297	C	O5'-P-OP2	-5.70	100.57	105.70
1	1A	1823	G	C8-N9-C1'	-5.70	119.58	127.00
1	1A	2774	C	N3-C4-C5	-5.70	119.62	121.90
32	1a	376	G	C4-N9-C1'	-5.70	119.08	126.50
32	1a	1523	G	N3-C4-C5	-5.70	125.75	128.60
1	2A	1151	G	C4-N9-C1'	-5.70	119.09	126.50
1	2A	1261	C	N1-C2-O2	-5.70	115.48	118.90
1	2A	2744	G	O5'-P-OP1	5.70	117.54	110.70
1	1A	1506	C	C5-C6-N1	5.70	123.85	121.00
1	1A	1963	U	OP1-P-OP2	5.70	128.15	119.60
1	1A	2603	G	N1-C6-O6	5.70	123.32	119.90
1	1A	2879	C	C4-C5-C6	5.70	120.25	117.40
32	1a	826	C	O5'-P-OP2	-5.70	100.57	105.70
1	2A	1611	C	O5'-P-OP1	-5.70	100.57	105.70
1	2A	198	C	N3-C4-C5	5.70	124.18	121.90
1	2A	498	G	N9-C4-C5	-5.70	103.12	105.40
1	2A	686	G	N1-C6-O6	-5.70	116.48	119.90
1	2A	1646	C	C2-N1-C1'	5.70	125.07	118.80
1	1A	2267	A	C6-N1-C2	-5.70	115.18	118.60
2	1B	13	A	N1-C6-N6	-5.70	115.18	118.60
32	1a	611	A	O5'-P-OP1	-5.70	100.57	105.70
32	1a	1354	C	C6-N1-C2	-5.70	118.02	120.30
32	1a	1486	G	C2-N3-C4	-5.70	109.05	111.90
1	2A	975(A)	G	N9-C4-C5	5.70	107.68	105.40
1	2A	2206	G	C4-N9-C1'	-5.70	119.09	126.50
1	1A	795	C	O5'-P-OP2	-5.70	100.57	105.70
1	1A	842	G	C8-N9-C4	5.70	108.68	106.40
1	1A	1825	A	C5-C6-N6	5.70	128.26	123.70
1	1A	2502	G	N9-C4-C5	5.70	107.68	105.40
1	1A	2766	G	N1-C2-N3	5.70	127.32	123.90
1	1A	381	G	N1-C2-N3	5.70	127.32	123.90
1	1A	732	C	N3-C4-N4	5.70	121.99	118.00
1	1A	796	C	C6-N1-C2	5.70	122.58	120.30
1	1A	906	G	O4'-C1'-N9	5.70	112.76	108.20
1	1A	1284	A	OP1-P-OP2	5.70	128.14	119.60
1	1A	2391	G	N1-C2-N3	5.70	127.32	123.90
32	1a	656	C	C5-C6-N1	5.70	123.85	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2428	G	C5-C6-N1	-5.70	108.65	111.50
1	2A	2677	G	C5-N7-C8	-5.70	101.45	104.30
32	2a	32	A	C6-N1-C2	-5.70	115.18	118.60
1	1A	2650	U	N3-C4-C5	5.69	118.02	114.60
1	2A	1047	G	N7-C8-N9	5.69	115.95	113.10
1	2A	2470	G	O5'-P-OP2	-5.69	100.58	105.70
32	2a	49	U	C2-N1-C1'	-5.69	110.87	117.70
1	1A	416	C	C6-N1-C2	5.69	122.58	120.30
1	1A	1125	G	C2-N3-C4	-5.69	109.05	111.90
1	1A	1668	A	C4-C5-C6	5.69	119.85	117.00
1	1A	1936	A	O5'-P-OP1	-5.69	100.58	105.70
1	1A	2142	C	C5-C6-N1	5.69	123.85	121.00
1	1A	2334	G	OP2-P-O3'	5.69	117.72	105.20
1	1A	2539	C	C2-N1-C1'	-5.69	112.54	118.80
1	1A	2838	G	N1-C6-O6	5.69	123.31	119.90
1	1A	2856	C	C5-C6-N1	5.69	123.85	121.00
32	1a	763	G	C8-N9-C4	-5.69	104.12	106.40
1	2A	389	G	C5-C6-O6	-5.69	125.18	128.60
1	2A	899	A	N1-C6-N6	-5.69	115.18	118.60
1	2A	1770	G	N9-C4-C5	5.69	107.68	105.40
1	2A	2575	C	C5-C6-N1	-5.69	118.15	121.00
1	1A	1251	C	OP1-P-OP2	5.69	128.13	119.60
1	1A	1643	G	N9-C4-C5	5.69	107.68	105.40
32	1a	1370	G	C2-N3-C4	-5.69	109.05	111.90
32	1a	1502	A	N1-C6-N6	-5.69	115.19	118.60
1	2A	956	G	N3-C2-N2	-5.69	115.92	119.90
1	2A	1864	U	C5-C4-O4	5.69	129.31	125.90
1	2A	2095	C	C6-N1-C2	-5.69	118.02	120.30
1	1A	813	U	N3-C4-O4	-5.69	115.42	119.40
1	1A	942	G	C8-N9-C4	5.69	108.67	106.40
1	1A	1555	G	N3-C2-N2	-5.69	115.92	119.90
1	1A	1823	G	C6-C5-N7	-5.69	126.99	130.40
1	1A	1959	G	C8-N9-C4	-5.69	104.12	106.40
32	1a	244	U	N1-C2-O2	5.69	126.78	122.80
1	2A	465	G	N3-C4-C5	-5.69	125.75	128.60
1	2A	1393	A	C8-N9-C4	5.69	108.08	105.80
32	2a	347	G	N3-C4-C5	5.69	131.44	128.60
32	2a	980	C	C5-C4-N4	-5.69	116.22	120.20
1	1A	845	G	O5'-P-OP2	-5.69	100.58	105.70
1	1A	1089	G	N3-C4-C5	-5.69	125.76	128.60
1	1A	1998	G	C5-C6-O6	5.69	132.01	128.60
1	1A	2303	G	N3-C4-N9	-5.69	122.59	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2607	G	N9-C4-C5	5.69	107.67	105.40
2	1B	32	C	O5'-P-OP1	-5.69	100.58	105.70
2	1B	50	G	C6-C5-N7	5.69	133.81	130.40
1	2A	792	G	N3-C4-C5	-5.69	125.76	128.60
1	1A	2417	C	N3-C4-C5	-5.69	119.63	121.90
32	2a	728	A	C4-C5-C6	5.69	119.84	117.00
1	1A	1762	A	C2-N3-C4	5.68	113.44	110.60
1	1A	1777	U	C6-N1-C2	5.68	124.41	121.00
32	1a	1480	G	C5-C6-N1	-5.68	108.66	111.50
1	2A	859	G	C2-N3-C4	-5.68	109.06	111.90
1	2A	1329	U	O5'-P-OP2	-5.68	100.58	105.70
1	2A	1353	A	C8-N9-C4	5.68	108.07	105.80
1	2A	2365	G	N9-C4-C5	-5.68	103.13	105.40
32	2a	24	U	N3-C2-O2	5.68	126.18	122.20
1	1A	375	C	C6-N1-C2	5.68	122.57	120.30
1	1A	394	A	N1-C2-N3	5.68	132.14	129.30
1	1A	689	A	C8-N9-C4	-5.68	103.53	105.80
1	1A	973	A	C4-C5-C6	5.68	119.84	117.00
1	1A	1655	A	C6-C5-N7	-5.68	128.32	132.30
1	1A	2841	C	C6-N1-C2	5.68	122.57	120.30
32	1a	455	C	N1-C2-O2	5.68	122.31	118.90
1	2A	329	G	C6-C5-N7	-5.68	126.99	130.40
1	2A	1926	U	C6-N1-C1'	5.68	129.16	121.20
32	2a	788	U	O5'-P-OP1	-5.68	100.59	105.70
32	1a	1442	G	P-O3'-C3'	5.68	126.52	119.70
1	2A	26	G	C4-C5-N7	5.68	113.07	110.80
1	2A	2622	C	N3-C4-C5	5.68	124.17	121.90
1	1A	127	A	N1-C2-N3	-5.68	126.46	129.30
1	1A	659	C	C2-N1-C1'	-5.68	112.55	118.80
1	1A	698	C	C5-C6-N1	-5.68	118.16	121.00
1	1A	724	U	C2-N1-C1'	-5.68	110.88	117.70
1	1A	1979	C	N3-C4-C5	5.68	124.17	121.90
1	2A	1479	G	N1-C6-O6	5.68	123.31	119.90
32	2a	530	G	N3-C2-N2	5.68	123.88	119.90
32	2a	649	G	C8-N9-C4	5.68	108.67	106.40
32	2a	1495	U	N3-C4-C5	-5.68	111.19	114.60
1	1A	645	C	C5-C6-N1	5.68	123.84	121.00
1	1A	2573	C	N3-C4-N4	5.68	121.97	118.00
1	2A	10	G	C4-C5-C6	-5.68	115.39	118.80
1	2A	614(B)	G	O4'-C1'-N9	5.68	112.74	108.20
1	1A	579	G	C4-C5-N7	5.68	113.07	110.80
1	1A	1796	U	C5-C6-N1	-5.68	119.86	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	803	G	C8-N9-C4	5.68	108.67	106.40
1	2A	298	G	N1-C6-O6	5.68	123.31	119.90
1	2A	686	G	C5-C6-N1	5.68	114.34	111.50
1	2A	1771	C	N3-C4-C5	5.68	124.17	121.90
1	1A	700	G	N7-C8-N9	5.67	115.94	113.10
1	1A	1146	C	N1-C2-O2	-5.67	115.50	118.90
1	1A	1438	U	C5-C4-O4	-5.67	122.50	125.90
1	1A	2202	C	O5'-P-OP2	-5.67	100.59	105.70
1	2A	271(S)	G	N7-C8-N9	5.67	115.94	113.10
1	2A	1469	A	C8-N9-C4	-5.67	103.53	105.80
1	2A	1963	U	O4'-C1'-N1	-5.67	103.66	108.20
1	2A	2032	G	C6-C5-N7	5.67	133.80	130.40
32	2a	297	G	C2-N3-C4	-5.67	109.06	111.90
32	2a	1301	U	C6-N1-C2	5.67	124.41	121.00
32	2a	1378	C	C6-N1-C2	-5.67	118.03	120.30
1	1A	792	G	N1-C2-N3	5.67	127.30	123.90
1	1A	827	U	N1-C2-N3	5.67	118.30	114.90
1	2A	1515	G	O5'-P-OP2	-5.67	100.59	105.70
1	1A	37	C	N3-C2-O2	-5.67	117.93	121.90
1	1A	975	C	O5'-P-OP2	5.67	117.50	110.70
1	1A	1563	G	OP2-P-O3'	5.67	117.68	105.20
1	1A	1877	A	OP2-P-O3'	5.67	117.68	105.20
1	2A	1348	G	OP1-P-O3'	5.67	117.67	105.20
1	2A	1385	G	N1-C6-O6	5.67	123.30	119.90
1	2A	1897	G	N3-C4-C5	5.67	131.44	128.60
32	2a	714	G	C5-C6-N1	-5.67	108.66	111.50
1	1A	99	U	C6-N1-C1'	-5.67	113.26	121.20
1	1A	179	G	C5-C6-N1	-5.67	108.67	111.50
1	1A	780	G	C5-N7-C8	5.67	107.14	104.30
1	1A	910	A	C5-C6-N6	-5.67	119.16	123.70
32	1a	977	A	N1-C6-N6	-5.67	115.20	118.60
32	1a	1184	G	N1-C6-O6	5.67	123.30	119.90
32	1a	1323	G	N1-C6-O6	5.67	123.30	119.90
1	2A	2695	C	C6-N1-C2	5.67	122.57	120.30
1	1A	2600	A	O5'-P-OP2	-5.67	100.60	105.70
1	1A	2747	G	C5-N7-C8	-5.67	101.47	104.30
32	2a	353	A	N1-C6-N6	5.67	122.00	118.60
32	2a	397	A	N7-C8-N9	5.67	116.63	113.80
1	1A	863	A	O5'-P-OP1	5.67	117.50	110.70
1	1A	912	C	C2-N1-C1'	5.67	125.03	118.80
1	1A	2406	U	C5-C4-O4	-5.67	122.50	125.90
32	1a	758	G	N3-C4-C5	5.67	131.43	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1356	G	C8-N9-C4	-5.67	104.13	106.40
1	2A	192	C	O5'-P-OP1	-5.67	100.60	105.70
1	2A	1026	U	N1-C2-O2	5.67	126.77	122.80
1	2A	1423	G	C8-N9-C4	5.67	108.67	106.40
32	2a	149	A	C8-N9-C4	-5.67	103.53	105.80
32	2a	241	C	N1-C2-O2	-5.67	115.50	118.90
1	1A	1060	U	C2-N1-C1'	5.67	124.50	117.70
1	1A	1615	C	C5-C4-N4	-5.67	116.23	120.20
1	1A	2276	G	N3-C2-N2	-5.67	115.93	119.90
1	2A	1647	G	N9-C4-C5	-5.67	103.13	105.40
1	2A	2040	C	N3-C4-N4	5.67	121.97	118.00
1	1A	510	C	OP1-P-O3'	5.66	117.66	105.20
1	1A	948	G	N1-C6-O6	5.66	123.30	119.90
1	1A	1225	G	O5'-P-OP2	5.66	117.50	110.70
1	1A	1385	G	N3-C4-N9	-5.66	122.60	126.00
1	1A	2031	A	N3-C4-C5	-5.66	122.83	126.80
1	1A	2314	C	C5-C6-N1	-5.66	118.17	121.00
1	1A	2554	U	C5-C4-O4	-5.66	122.50	125.90
1	1A	2823	A	C2-N3-C4	-5.66	107.77	110.60
1	2A	2517	C	O4'-C1'-N1	5.66	112.73	108.20
32	2a	324	G	N1-C6-O6	5.66	123.30	119.90
1	1A	318	C	N3-C4-C5	-5.66	119.64	121.90
1	1A	2357	U	O5'-P-OP1	5.66	117.49	110.70
1	1A	2380	C	N3-C4-C5	5.66	124.17	121.90
32	2a	353	A	C4-C5-N7	5.66	113.53	110.70
32	2a	481	G	C6-C5-N7	-5.66	127.00	130.40
1	1A	218	A	C5-C6-N6	5.66	128.23	123.70
1	1A	272(H)	C	N3-C4-C5	5.66	124.16	121.90
1	1A	1105	U	N3-C2-O2	5.66	126.16	122.20
1	1A	1417	C	C6-N1-C2	5.66	122.56	120.30
1	1A	1955	U	OP1-P-OP2	5.66	128.09	119.60
1	1A	1969	A	O5'-P-OP2	5.66	117.49	110.70
1	1A	2501	C	O5'-P-OP1	-5.66	100.61	105.70
2	1B	60	C	C5-C6-N1	5.66	123.83	121.00
1	2A	615	G	C8-N9-C4	5.66	108.66	106.40
1	2A	956	G	C6-C5-N7	-5.66	127.00	130.40
1	2A	1325	G	C4-C5-N7	5.66	113.06	110.80
1	2A	2032	G	C4-C5-N7	-5.66	108.54	110.80
1	2A	2177	C	C2-N1-C1'	5.66	125.03	118.80
1	2A	2385	C	OP1-P-OP2	5.66	128.09	119.60
1	2A	2427	C	C2-N1-C1'	-5.66	112.57	118.80
1	1A	792	G	O5'-P-OP1	-5.66	100.61	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2078	C	N3-C4-C5	-5.66	119.64	121.90
32	2a	485	G	C4-C5-N7	-5.66	108.54	110.80
1	1A	1344	G	N1-C6-O6	5.66	123.29	119.90
1	1A	2705	A	C4-C5-C6	5.66	119.83	117.00
2	1B	105	A	C5-C6-N6	-5.66	119.17	123.70
1	1A	558	G	C8-N9-C4	5.66	108.66	106.40
1	1A	1011	G	C5-N7-C8	5.66	107.13	104.30
1	1A	1994	C	OP1-P-OP2	-5.66	111.12	119.60
32	1a	921	U	C5-C6-N1	5.66	125.53	122.70
1	2A	727	A	OP2-P-O3'	5.66	117.64	105.20
1	2A	1325	G	N3-C4-C5	-5.66	125.77	128.60
1	2A	1391	U	O5'-P-OP2	5.66	117.49	110.70
1	2A	1617	C	C2-N1-C1'	5.66	125.02	118.80
1	2A	2056	G	C5-C6-O6	-5.66	125.21	128.60
32	2a	326	G	C4-C5-N7	-5.66	108.54	110.80
32	2a	522	C	C4-C5-C6	5.66	120.23	117.40
1	1A	399	G	N1-C6-O6	5.65	123.29	119.90
1	2A	1421	G	N1-C6-O6	5.65	123.29	119.90
32	2a	1301	U	C2-N1-C1'	-5.65	110.92	117.70
1	1A	475	U	C4-C5-C6	5.65	123.09	119.70
1	1A	484	C	N3-C2-O2	5.65	125.86	121.90
1	1A	1546	C	C6-N1-C2	5.65	122.56	120.30
1	1A	1913	A	N1-C6-N6	-5.65	115.21	118.60
1	1A	2856	C	C6-N1-C2	-5.65	118.04	120.30
32	1a	266	G	C4-N9-C1'	5.65	133.85	126.50
32	1a	491	G	C4-N9-C1'	-5.65	119.15	126.50
1	2A	784	A	OP2-P-O3'	5.65	117.63	105.20
1	1A	135	G	C2-N3-C4	-5.65	109.08	111.90
1	1A	1607	C	N3-C2-O2	-5.65	117.94	121.90
1	1A	1854	A	C5-N7-C8	-5.65	101.08	103.90
2	1B	17	C	C5-C6-N1	-5.65	118.17	121.00
32	1a	1530	G	C6-C5-N7	-5.65	127.01	130.40
1	2A	388	G	N3-C4-N9	-5.65	122.61	126.00
1	2A	772	C	OP2-P-O3'	5.65	117.63	105.20
1	2A	783	A	N9-C4-C5	5.65	108.06	105.80
1	2A	945	A	C8-N9-C4	5.65	108.06	105.80
1	2A	1247	A	C2-N3-C4	-5.65	107.77	110.60
1	2A	1415	U	C5-C6-N1	-5.65	119.88	122.70
1	2A	2371	G	C6-N1-C2	-5.65	121.71	125.10
32	1a	330	C	C6-N1-C2	-5.65	118.04	120.30
1	2A	687	C	C4-C5-C6	5.65	120.22	117.40
1	2A	2445	G	N3-C4-C5	-5.65	125.78	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	26	G	C6-C5-N7	-5.65	127.01	130.40
1	1A	250	G	C5-C6-N1	-5.65	108.68	111.50
1	1A	684	G	C5-C6-N1	5.65	114.32	111.50
1	1A	873	G	OP2-P-O3'	5.65	117.62	105.20
1	1A	2562	U	C5-C6-N1	-5.65	119.88	122.70
1	1A	2743	C	C4-C5-C6	5.65	120.22	117.40
2	1B	82	G	C2-N3-C4	-5.65	109.08	111.90
32	1a	1516	G	N1-C2-N2	5.65	121.28	116.20
1	2A	80	G	C5-C6-O6	5.65	131.99	128.60
1	2A	488	G	O5'-P-OP2	-5.65	100.62	105.70
1	2A	1381	G	N3-C4-N9	-5.65	122.61	126.00
1	2A	1471	A	C4-N9-C1'	5.65	136.47	126.30
1	2A	1796	U	N1-C2-O2	-5.65	118.85	122.80
1	2A	1280	G	OP2-P-O3'	5.65	117.62	105.20
1	2A	2421	G	C8-N9-C1'	-5.65	119.66	127.00
1	2A	2520	C	C6-N1-C2	5.65	122.56	120.30
1	1A	1192	G	N1-C6-O6	5.64	123.29	119.90
1	1A	2011	U	O5'-P-OP1	-5.64	100.62	105.70
1	1A	2465	C	O5'-P-OP2	-5.64	100.62	105.70
1	1A	2730	C	C2-N3-C4	-5.64	117.08	119.90
2	1B	79	C	N3-C2-O2	-5.64	117.95	121.90
32	1a	487	A	C8-N9-C4	5.64	108.06	105.80
1	2A	363	G	N3-C4-C5	5.64	131.42	128.60
1	2A	795	C	C6-N1-C2	-5.64	118.04	120.30
1	2A	973	A	N7-C8-N9	5.64	116.62	113.80
1	2A	1268	A	N1-C2-N3	5.64	132.12	129.30
1	2A	2581	G	C4-N9-C1'	5.64	133.84	126.50
1	1A	1328	G	N3-C4-N9	5.64	129.38	126.00
1	1A	1411	C	C5-C6-N1	-5.64	118.18	121.00
32	1a	572	A	C4-N9-C1'	-5.64	116.14	126.30
32	1a	764	C	C6-N1-C2	-5.64	118.04	120.30
1	2A	1494	A	C5-C6-N1	-5.64	114.88	117.70
1	1A	677	A	C4-C5-C6	5.64	119.82	117.00
1	1A	757	U	N3-C2-O2	-5.64	118.25	122.20
14	1S	9	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	2A	646	A	C8-N9-C4	-5.64	103.54	105.80
1	2A	1991	U	N3-C4-C5	5.64	117.98	114.60
1	2A	2133	G	N7-C8-N9	-5.64	110.28	113.10
1	2A	2163	C	N1-C2-O2	5.64	122.28	118.90
1	1A	472	A	N1-C6-N6	5.64	121.98	118.60
1	1A	529	A	N9-C4-C5	-5.64	103.55	105.80
1	1A	622	G	N1-C2-N2	-5.64	111.12	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1025	G	N7-C8-N9	-5.64	110.28	113.10
1	1A	1132	A	C6-N1-C2	-5.64	115.22	118.60
1	1A	1991	U	C5-C6-N1	-5.64	119.88	122.70
1	1A	2509	G	C5-N7-C8	-5.64	101.48	104.30
1	2A	146	G	C8-N9-C4	5.64	108.66	106.40
1	2A	263	C	C5-C6-N1	-5.64	118.18	121.00
1	2A	1788	C	O5'-P-OP2	5.64	117.47	110.70
1	2A	1835	G	N1-C2-N3	5.64	127.28	123.90
32	1a	783	C	C5-C6-N1	-5.64	118.18	121.00
32	1a	1158	C	C4-C5-C6	5.64	120.22	117.40
1	2A	690	G	C5-C6-O6	-5.64	125.22	128.60
1	2A	2565	A	C4-C5-N7	-5.64	107.88	110.70
32	2a	1442	G	N3-C4-N9	5.64	129.38	126.00
1	1A	224	G	C5-N7-C8	5.64	107.12	104.30
1	1A	976	C	C5-C6-N1	5.64	123.82	121.00
1	1A	978	G	N3-C4-C5	5.64	131.42	128.60
1	1A	1170	G	C6-C5-N7	-5.64	127.02	130.40
1	1A	2351	G	OP2-P-O3'	5.64	117.60	105.20
1	1A	2358	G	N3-C2-N2	-5.64	115.95	119.90
1	2A	741	G	C6-C5-N7	5.64	133.78	130.40
1	2A	1205	U	N3-C4-C5	-5.64	111.22	114.60
1	1A	651	G	C2-N3-C4	5.63	114.72	111.90
1	1A	1234	U	C5-C6-N1	-5.63	119.88	122.70
1	1A	2392	A	C5-C6-N1	-5.63	114.88	117.70
1	1A	2717	G	C6-C5-N7	-5.63	127.02	130.40
32	1a	1504	G	C8-N9-C4	5.63	108.65	106.40
1	2A	10	G	C4-N9-C1'	-5.63	119.17	126.50
1	2A	582	G	C2-N3-C4	-5.63	109.08	111.90
1	2A	698	C	C5-C6-N1	-5.63	118.18	121.00
1	2A	731	C	N1-C2-O2	5.63	122.28	118.90
1	2A	1206	G	N1-C6-O6	5.63	123.28	119.90
1	2A	1691	C	C6-N1-C2	-5.63	118.05	120.30
1	2A	1776	G	O5'-P-OP1	5.63	117.46	110.70
1	2A	1891	G	N3-C4-N9	-5.63	122.62	126.00
2	2B	102	A	N9-C4-C5	-5.63	103.55	105.80
32	2a	721	G	C4-C5-C6	5.63	122.18	118.80
32	2a	816	A	O5'-P-OP1	5.63	117.46	110.70
1	1A	2028	U	N3-C4-O4	-5.63	115.46	119.40
1	1A	2507	C	N3-C2-O2	5.63	125.84	121.90
1	1A	2696	U	N1-C2-O2	5.63	126.74	122.80
32	1a	1053	G	C5-C6-O6	-5.63	125.22	128.60
1	2A	2004	G	C5-C6-O6	5.63	131.98	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2B	23	G	C5-C6-O6	-5.63	125.22	128.60
1	1A	677	A	OP1-P-O3'	5.63	117.59	105.20
1	1A	1310	G	C5-C6-N1	5.63	114.32	111.50
1	1A	1383	C	N1-C2-O2	-5.63	115.52	118.90
1	1A	2250	G	C6-C5-N7	5.63	133.78	130.40
1	1A	2446	G	OP2-P-O3'	5.63	117.59	105.20
1	1A	2775	A	C6-N1-C2	-5.63	115.22	118.60
1	2A	252	G	C6-C5-N7	5.63	133.78	130.40
1	2A	2032	G	C8-N9-C4	5.63	108.65	106.40
32	2a	120	A	N9-C4-C5	5.63	108.05	105.80
32	2a	879	C	N3-C2-O2	-5.63	117.96	121.90
1	1A	1618	A	O5'-P-OP1	-5.63	100.63	105.70
1	1A	1674	G	C8-N9-C4	5.63	108.65	106.40
1	1A	2733	A	N1-C6-N6	5.63	121.98	118.60
32	1a	53	A	N1-C6-N6	-5.63	115.22	118.60
1	2A	751	A	O5'-P-OP2	5.63	117.46	110.70
1	2A	2458	G	C6-N1-C2	-5.63	121.72	125.10
2	2B	24	G	N1-C6-O6	5.63	123.28	119.90
32	2a	421	U	C6-N1-C1'	-5.63	113.32	121.20
32	2a	442	C	C2-N1-C1'	5.63	124.99	118.80
1	1A	1197	G	N9-C4-C5	-5.63	103.15	105.40
1	1A	1830	C	C2-N3-C4	-5.63	117.09	119.90
1	1A	2278	A	OP2-P-O3'	5.63	117.58	105.20
1	1A	2278	A	O4'-C1'-N9	-5.63	103.70	108.20
1	1A	2712	U	C5-C4-O4	-5.63	122.52	125.90
1	1A	2840	C	C6-N1-C2	-5.63	118.05	120.30
1	2A	468	G	O5'-P-OP2	5.63	117.45	110.70
1	2A	1547	C	C4-C5-C6	5.63	120.21	117.40
2	2B	78	A	C5-C6-N6	-5.63	119.20	123.70
1	1A	54	G	N1-C6-O6	5.63	123.28	119.90
1	1A	1015	G	O5'-P-OP1	5.63	117.45	110.70
1	1A	1092	C	C4-C5-C6	-5.63	114.59	117.40
1	1A	1239	G	C5-N7-C8	-5.63	101.49	104.30
1	1A	1270	C	N3-C4-C5	5.63	124.15	121.90
1	1A	1699	G	C8-N9-C4	-5.63	104.15	106.40
32	1a	330	C	C5-C6-N1	5.63	123.81	121.00
32	1a	722	A	C2-N3-C4	-5.63	107.79	110.60
32	1a	1403	C	O5'-P-OP2	-5.63	100.64	105.70
1	2A	247	G	C8-N9-C4	5.63	108.65	106.40
1	2A	692	C	N1-C2-O2	-5.63	115.53	118.90
1	2A	759	G	O5'-P-OP1	-5.63	100.64	105.70
1	2A	1109	C	C6-N1-C1'	-5.63	114.05	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2662	A	N1-C6-N6	5.63	121.98	118.60
1	1A	1397	U	OP1-P-OP2	-5.62	111.16	119.60
32	2a	1028	C	C6-N1-C2	-5.62	118.05	120.30
1	1A	1439	A	C2-N3-C4	-5.62	107.79	110.60
1	1A	2068	U	N3-C4-O4	5.62	123.34	119.40
1	1A	2255	G	O5'-P-OP2	-5.62	100.64	105.70
1	1A	2591	C	OP1-P-O3'	5.62	117.57	105.20
1	2A	529	A	C5-N7-C8	-5.62	101.09	103.90
32	2a	729	A	N7-C8-N9	5.62	116.61	113.80
32	2a	932	C	C6-N1-C2	-5.62	118.05	120.30
1	1A	27	G	N9-C4-C5	-5.62	103.15	105.40
1	1A	794	G	N1-C6-O6	-5.62	116.53	119.90
1	1A	1257	C	N3-C4-C5	-5.62	119.65	121.90
1	1A	1494	A	N7-C8-N9	5.62	116.61	113.80
1	1A	1800	C	N3-C2-O2	-5.62	117.97	121.90
1	1A	2872	G	C6-N1-C2	-5.62	121.73	125.10
32	1a	1435	G	N3-C4-N9	-5.62	122.63	126.00
32	1a	1457	G	C8-N9-C4	5.62	108.65	106.40
32	1a	1529	G	O4'-C1'-N9	5.62	112.70	108.20
1	2A	10	G	C5-C6-O6	-5.62	125.23	128.60
1	2A	1076	C	N3-C2-O2	-5.62	117.97	121.90
1	2A	1965	C	C4-C5-C6	-5.62	114.59	117.40
32	2a	1054	C	O5'-P-OP2	-5.62	100.64	105.70
1	1A	2026	C	O5'-P-OP1	5.62	117.44	110.70
1	1A	2130	U	C6-N1-C2	-5.62	117.63	121.00
1	1A	2327	A	C6-N1-C2	-5.62	115.23	118.60
1	2A	1325	G	C6-N1-C2	-5.62	121.73	125.10
1	1A	1220	A	N9-C4-C5	5.62	108.05	105.80
1	1A	1261	C	C5-C6-N1	-5.62	118.19	121.00
1	1A	2015	A	O5'-P-OP1	-5.62	100.64	105.70
1	1A	2037	G	N9-C4-C5	-5.62	103.15	105.40
32	1a	801	U	N3-C4-O4	-5.62	115.47	119.40
32	1a	1265	G	N9-C4-C5	-5.62	103.15	105.40
41	1j	9	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	2A	906	G	C4-C5-N7	-5.62	108.55	110.80
1	2A	214	G	C4-N9-C1'	-5.62	119.20	126.50
1	2A	383	U	C5-C4-O4	5.62	129.27	125.90
1	2A	1628	G	C8-N9-C4	5.62	108.65	106.40
32	2a	472	A	N7-C8-N9	5.62	116.61	113.80
1	1A	403	U	N3-C2-O2	-5.62	118.27	122.20
1	1A	620	G	OP1-P-OP2	5.62	128.02	119.60
1	1A	1162	G	C4-C5-N7	-5.62	108.55	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2191	G	C5-C6-O6	-5.62	125.23	128.60
1	2A	125	G	C5-C6-O6	-5.62	125.23	128.60
1	2A	420	C	C2-N1-C1'	-5.62	112.62	118.80
1	2A	819	A	N7-C8-N9	5.62	116.61	113.80
1	2A	2182	G	C4-C5-N7	-5.62	108.55	110.80
1	2A	2508	G	C5-C6-N1	5.62	114.31	111.50
1	2A	2816	C	N3-C4-C5	-5.62	119.65	121.90
32	2a	722	A	N1-C6-N6	5.62	121.97	118.60
1	1A	753	C	O5'-P-OP2	-5.61	100.65	105.70
1	1A	1969	A	C2-N3-C4	-5.61	107.79	110.60
1	2A	964	C	C6-N1-C2	-5.61	118.06	120.30
1	1A	1342	A	C4-C5-N7	5.61	113.51	110.70
1	1A	1785	A	C2-N3-C4	5.61	113.41	110.60
1	1A	1981	A	N9-C4-C5	5.61	108.05	105.80
1	2A	824	A	N1-C2-N3	-5.61	126.49	129.30
1	2A	2009	G	N7-C8-N9	-5.61	110.29	113.10
1	2A	2751	G	N1-C6-O6	-5.61	116.53	119.90
32	2a	1492	A	C8-N9-C4	-5.61	103.56	105.80
1	1A	223	A	OP1-P-OP2	5.61	128.02	119.60
1	1A	591	C	N1-C2-O2	-5.61	115.53	118.90
1	1A	1003	G	C5-N7-C8	5.61	107.11	104.30
1	1A	1789	A	N9-C4-C5	-5.61	103.56	105.80
2	1B	27	C	C4-C5-C6	5.61	120.20	117.40
1	2A	501	A	C5-C6-N1	-5.61	114.89	117.70
1	2A	1693	U	OP1-P-OP2	5.61	128.02	119.60
1	2A	1935	G	C5-N7-C8	-5.61	101.50	104.30
1	2A	2084	C	N1-C2-N3	-5.61	115.27	119.20
1	1A	679	C	C5-C6-N1	-5.61	118.20	121.00
1	1A	1665	A	OP1-P-O3'	5.61	117.53	105.20
1	1A	1853	A	C4-C5-N7	-5.61	107.90	110.70
1	1A	2428	G	C4-C5-N7	5.61	113.04	110.80
1	1A	2701	C	C5-C6-N1	-5.61	118.20	121.00
1	2A	1009	A	OP1-P-OP2	-5.61	111.19	119.60
1	2A	1678	G	C8-N9-C4	-5.61	104.16	106.40
1	2A	2491	U	C5-C6-N1	5.61	125.50	122.70
32	2a	226	G	N7-C8-N9	-5.61	110.30	113.10
32	2a	698	G	C5-C6-O6	-5.61	125.24	128.60
1	1A	513	A	C4-C5-C6	5.61	119.80	117.00
1	1A	513	A	C6-C5-N7	-5.61	128.38	132.30
1	1A	568	U	C2-N3-C4	-5.61	123.64	127.00
1	1A	720	C	C6-N1-C2	5.61	122.54	120.30
1	1A	726	G	OP1-P-OP2	5.61	128.01	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	271(S)	G	N1-C6-O6	5.61	123.26	119.90
1	2A	1184	G	C4-C5-N7	5.61	113.04	110.80
1	2A	2394	C	C4-C5-C6	5.61	120.20	117.40
32	2a	656	C	OP2-P-O3'	5.61	117.53	105.20
32	2a	1486	G	O5'-P-OP1	5.61	117.43	110.70
1	1A	993	G	C4-N9-C1'	-5.60	119.22	126.50
1	1A	2782	G	N9-C4-C5	-5.60	103.16	105.40
32	1a	1134	G	C8-N9-C4	-5.60	104.16	106.40
1	2A	129	C	O5'-P-OP2	-5.60	100.66	105.70
1	2A	2449	U	C5-C4-O4	-5.60	122.54	125.90
32	2a	1137	C	N3-C4-C5	-5.60	119.66	121.90
32	2a	1397	C	N1-C2-O2	5.60	122.26	118.90
1	1A	579	G	C5-N7-C8	-5.60	101.50	104.30
1	1A	1705	G	C2-N3-C4	-5.60	109.10	111.90
32	1a	323	U	C5-C6-N1	5.60	125.50	122.70
1	2A	2439	A	N1-C2-N3	5.60	132.10	129.30
2	2B	118	G	N1-C6-O6	-5.60	116.54	119.90
1	1A	60	G	O5'-P-OP1	-5.60	100.66	105.70
32	1a	1112	C	C6-N1-C2	-5.60	118.06	120.30
1	2A	2606	C	C6-N1-C1'	5.60	127.52	120.80
1	2A	2616	C	C2-N3-C4	-5.60	117.10	119.90
1	2A	2791	C	N3-C2-O2	-5.60	117.98	121.90
32	2a	621	A	C8-N9-C4	-5.60	103.56	105.80
1	1A	2644	G	N3-C2-N2	-5.60	115.98	119.90
1	2A	330	A	N9-C1'-C2'	-5.60	105.84	112.00
1	2A	762	U	C6-N1-C1'	-5.60	113.36	121.20
1	2A	1127	A	C8-N9-C4	-5.60	103.56	105.80
1	2A	1176	G	P-O3'-C3'	5.60	126.42	119.70
1	2A	1328	G	C5-C6-N1	5.60	114.30	111.50
1	2A	2685	G	C6-C5-N7	5.60	133.76	130.40
1	2A	2763	G	N3-C4-N9	5.60	129.36	126.00
2	2B	60	C	N1-C2-O2	5.60	122.26	118.90
32	2a	1274	G	N7-C8-N9	5.60	115.90	113.10
1	1A	312	G	O5'-P-OP2	5.60	117.42	110.70
1	1A	2582	G	N3-C4-C5	-5.60	125.80	128.60
1	1A	2599	G	N3-C2-N2	-5.60	115.98	119.90
2	1B	106	G	C2-N3-C4	5.60	114.70	111.90
32	1a	1003	G	C2-N3-C4	5.60	114.70	111.90
1	2A	652(A)	A	N3-C4-C5	-5.60	122.88	126.80
1	2A	2407	G	C8-N9-C1'	-5.60	119.72	127.00
32	2a	117	G	N9-C4-C5	-5.60	103.16	105.40
1	1A	37	C	OP2-P-O3'	5.60	117.51	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	141	A	N9-C4-C5	5.60	108.04	105.80
1	2A	614(C)	A	N7-C8-N9	5.60	116.60	113.80
1	2A	1262	A	N7-C8-N9	5.60	116.60	113.80
1	1A	857	C	OP1-P-OP2	5.59	127.99	119.60
1	1A	1046	A	N3-C4-C5	-5.59	122.88	126.80
1	1A	1815	A	C5-C6-N1	5.59	120.50	117.70
32	1a	282	A	OP1-P-OP2	-5.59	111.21	119.60
32	1a	1137	C	C6-N1-C1'	5.59	127.51	120.80
1	2A	620	G	C2-N3-C4	5.59	114.70	111.90
1	2A	1378	A	O5'-P-OP1	-5.59	100.67	105.70
1	2A	1494	A	C4-C5-C6	5.59	119.80	117.00
1	1A	195	A	OP1-P-O3'	-5.59	92.89	105.20
1	1A	793	A	C2-N3-C4	-5.59	107.80	110.60
1	1A	1255	U	N3-C2-O2	-5.59	118.28	122.20
1	2A	1287	A	C5-N7-C8	-5.59	101.10	103.90
1	2A	1337	G	N9-C1'-C2'	-5.59	105.85	112.00
1	1A	854	G	O5'-P-OP1	5.59	117.41	110.70
1	1A	1005	C	O5'-P-OP2	-5.59	100.67	105.70
1	1A	1236	G	C5-C6-O6	-5.59	125.25	128.60
1	1A	2238	G	O5'-P-OP2	-5.59	100.67	105.70
32	1a	453	A	C8-N9-C4	-5.59	103.56	105.80
32	1a	498	U	C5-C4-O4	5.59	129.25	125.90
1	2A	446	G	N1-C6-O6	5.59	123.25	119.90
1	2A	932	G	C8-N9-C1'	5.59	134.27	127.00
1	2A	1781	C	C2-N1-C1'	-5.59	112.65	118.80
1	2A	1927	A	C5-N7-C8	-5.59	101.10	103.90
32	2a	898	G	C5-C6-O6	-5.59	125.25	128.60
1	1A	54	G	C2-N3-C4	-5.59	109.11	111.90
1	1A	641	C	N1-C2-O2	-5.59	115.55	118.90
1	1A	768	G	C4-C5-N7	5.59	113.04	110.80
1	1A	843	G	C2-N3-C4	-5.59	109.11	111.90
1	1A	958	U	N1-C2-O2	-5.59	118.89	122.80
1	1A	1053	C	N1-C1'-C2'	-5.59	105.85	112.00
1	1A	1239	G	N7-C8-N9	5.59	115.89	113.10
1	1A	2178	C	C6-N1-C2	-5.59	118.06	120.30
1	1A	2820	A	C5-C6-N1	-5.59	114.91	117.70
32	1a	852	G	C5-C6-N1	-5.59	108.70	111.50
1	2A	845	G	N3-C4-C5	-5.59	125.81	128.60
1	2A	1812	A	C8-N9-C4	-5.59	103.56	105.80
1	2A	1840	G	N1-C2-N3	-5.59	120.55	123.90
1	2A	2373	G	OP1-P-OP2	5.59	127.98	119.60
1	1A	1248	G	O5'-P-OP1	5.59	117.41	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1447	G	N3-C4-N9	-5.59	122.65	126.00
1	1A	2607	G	C5-C6-O6	5.59	131.95	128.60
1	1A	642	G	O5'-P-OP1	5.59	117.41	110.70
1	1A	714	U	N1-C2-N3	5.59	118.25	114.90
1	1A	1566	A	C4-N9-C1'	-5.59	116.24	126.30
1	1A	2837	G	C5-C6-O6	-5.59	125.25	128.60
2	1B	84	C	C6-N1-C2	-5.59	118.07	120.30
32	1a	437	U	OP2-P-O3'	5.59	117.49	105.20
1	2A	206	U	C2-N1-C1'	5.59	124.40	117.70
1	2A	2407	G	N9-C4-C5	-5.59	103.17	105.40
32	2a	1432	G	C4-C5-N7	-5.59	108.56	110.80
1	1A	1616	A	C5-N7-C8	-5.58	101.11	103.90
1	1A	2429	G	OP1-P-OP2	-5.58	111.22	119.60
1	1A	2487	G	C6-C5-N7	-5.58	127.05	130.40
1	2A	2818	G	C5-C6-O6	5.58	131.95	128.60
32	2a	1375	A	C8-N9-C4	-5.58	103.57	105.80
1	1A	768	G	N1-C2-N3	5.58	127.25	123.90
1	1A	955	C	C5-C6-N1	-5.58	118.21	121.00
1	1A	1696	G	N1-C6-O6	-5.58	116.55	119.90
1	1A	2286	A	O5'-P-OP1	5.58	117.40	110.70
1	1A	2329	G	N3-C4-C5	5.58	131.39	128.60
1	2A	1004	C	N3-C4-C5	-5.58	119.67	121.90
1	2A	1996	C	OP1-P-O3'	5.58	117.48	105.20
1	2A	2504	U	C5-C6-N1	5.58	125.49	122.70
1	2A	2565	A	N1-C6-N6	-5.58	115.25	118.60
32	2a	1048	G	C8-N9-C4	-5.58	104.17	106.40
1	1A	1206	G	C6-N1-C2	-5.58	121.75	125.10
1	2A	569	U	N1-C2-O2	-5.58	118.89	122.80
1	2A	695	G	C8-N9-C4	5.58	108.63	106.40
1	2A	948	G	N1-C6-O6	5.58	123.25	119.90
1	2A	2076	U	C5-C6-N1	5.58	125.49	122.70
32	2a	220	G	C4-N9-C1'	5.58	133.76	126.50
32	2a	525	C	N1-C2-N3	-5.58	115.29	119.20
32	2a	890	G	C8-N9-C4	-5.58	104.17	106.40
1	1A	660	G	C6-N1-C2	5.58	128.45	125.10
1	1A	1410	G	C2-N3-C4	-5.58	109.11	111.90
2	1B	103	G	N3-C4-N9	-5.58	122.65	126.00
1	2A	2722	G	O5'-P-OP1	-5.58	100.68	105.70
1	1A	608	A	C6-C5-N7	-5.58	128.40	132.30
1	1A	1014	U	N1-C2-N3	5.58	118.25	114.90
1	1A	2288	A	N1-C6-N6	5.58	121.95	118.60
1	1A	2496	C	OP1-P-O3'	5.58	117.47	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1444	C	C6-N1-C2	5.58	122.53	120.30
1	2A	684	G	N7-C8-N9	5.58	115.89	113.10
1	2A	738	G	C5-N7-C8	5.58	107.09	104.30
1	2A	1338	G	OP1-P-O3'	5.58	117.47	105.20
1	2A	2177	C	C6-N1-C2	-5.58	118.07	120.30
32	2a	550	G	C4-N9-C1'	-5.58	119.25	126.50
32	2a	730	G	C6-C5-N7	5.58	133.75	130.40
1	1A	1847	A	C8-N9-C1'	-5.58	117.66	127.70
1	1A	2520	C	P-O3'-C3'	-5.58	113.01	119.70
32	1a	325	A	N9-C4-C5	-5.58	103.57	105.80
32	1a	1479	C	N3-C2-O2	5.58	125.80	121.90
32	2a	1486	G	C5-C6-O6	-5.58	125.25	128.60
1	1A	1995	U	N3-C2-O2	5.58	126.10	122.20
2	1B	53	A	N7-C8-N9	5.58	116.59	113.80
1	2A	18	C	C6-N1-C2	-5.58	118.07	120.30
1	2A	65	C	C6-N1-C2	-5.58	118.07	120.30
1	2A	98	G	N3-C4-C5	5.58	131.39	128.60
1	2A	172	C	C6-N1-C2	-5.58	118.07	120.30
1	2A	773	U	N1-C2-O2	-5.58	118.90	122.80
1	2A	1213	A	N1-C6-N6	5.58	121.94	118.60
1	2A	2191	G	C4-C5-N7	5.58	113.03	110.80
1	2A	2650	U	N3-C2-O2	5.58	126.10	122.20
1	1A	737	C	C5-C6-N1	-5.57	118.21	121.00
1	1A	756	C	C4-C5-C6	5.57	120.19	117.40
1	1A	1394	U	N3-C2-O2	-5.57	118.30	122.20
1	1A	2646	C	N1-C2-O2	-5.57	115.56	118.90
1	1A	2739	U	C5-C6-N1	-5.57	119.91	122.70
32	1a	731	G	N3-C2-N2	-5.57	116.00	119.90
1	2A	1625	C	O5'-P-OP2	-5.57	100.68	105.70
1	2A	2710	C	C6-N1-C2	-5.57	118.07	120.30
1	1A	213	A	OP2-P-O3'	5.57	117.46	105.20
1	1A	690	G	N9-C4-C5	-5.57	103.17	105.40
1	1A	2501	C	C2-N1-C1'	-5.57	112.67	118.80
32	1a	719	C	C6-N1-C2	-5.57	118.07	120.30
1	2A	399	G	C5-N7-C8	-5.57	101.51	104.30
1	1A	206	U	C4-C5-C6	5.57	123.04	119.70
1	1A	708	C	N3-C2-O2	-5.57	118.00	121.90
1	1A	1621	U	OP1-P-O3'	5.57	117.46	105.20
1	1A	2269	A	C6-C5-N7	-5.57	128.40	132.30
1	2A	259	G	C8-N9-C4	-5.57	104.17	106.40
1	1A	2069	G	N9-C4-C5	5.57	107.63	105.40
1	2A	1682	G	C8-N9-C4	5.57	108.63	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	657	G	C5-C6-N1	-5.57	108.72	111.50
1	1A	106	C	N3-C2-O2	5.57	125.80	121.90
1	1A	794	G	OP1-P-OP2	-5.57	111.25	119.60
1	1A	911	A	OP1-P-OP2	5.57	127.95	119.60
1	1A	1272	A	C4-C5-C6	5.57	119.78	117.00
1	1A	1608	A	OP2-P-O3'	5.57	117.45	105.20
1	1A	1792	G	N1-C2-N2	5.57	121.21	116.20
1	1A	2690	C	O5'-P-OP1	-5.57	100.69	105.70
1	2A	457	A	C8-N9-C4	-5.57	103.57	105.80
1	2A	2658	C	O5'-P-OP1	-5.57	100.69	105.70
32	2a	329	A	N1-C2-N3	5.57	132.08	129.30
1	1A	2050	C	O5'-P-OP2	-5.57	100.69	105.70
1	1A	2417	C	C4-C5-C6	5.57	120.18	117.40
2	1B	91	C	N3-C4-C5	5.57	124.13	121.90
32	1a	803	G	N9-C4-C5	-5.57	103.17	105.40
32	1a	804	U	C2-N1-C1'	-5.57	111.02	117.70
1	2A	189	G	C5-N7-C8	5.57	107.08	104.30
1	2A	1817	G	C6-C5-N7	5.57	133.74	130.40
1	2A	1820	U	C6-N1-C1'	-5.57	113.41	121.20
1	2A	2073	C	C5-C6-N1	5.57	123.78	121.00
32	2a	698	G	C4-C5-N7	5.57	113.03	110.80
32	2a	792	A	N1-C6-N6	5.57	121.94	118.60
1	1A	307	G	C6-C5-N7	-5.56	127.06	130.40
1	1A	2032	G	C2-N3-C4	-5.56	109.12	111.90
32	2a	511	C	C2-N1-C1'	-5.56	112.68	118.80
1	1A	213	A	C4-C5-N7	5.56	113.48	110.70
1	1A	1280	G	OP1-P-OP2	-5.56	111.26	119.60
1	1A	2056	G	C5-N7-C8	-5.56	101.52	104.30
1	2A	194	G	C5-C6-O6	-5.56	125.26	128.60
1	2A	690	G	O5'-P-OP2	-5.56	100.69	105.70
1	2A	773	U	C4-C5-C6	5.56	123.04	119.70
32	2a	754	C	C2-N1-C1'	5.56	124.92	118.80
1	1A	1234	U	N1-C2-N3	5.56	118.24	114.90
1	2A	2513	G	C5-N7-C8	-5.56	101.52	104.30
1	1A	301	G	OP1-P-OP2	5.56	127.94	119.60
1	1A	933	A	C4-C5-C6	5.56	119.78	117.00
1	1A	1135	C	N3-C2-O2	-5.56	118.01	121.90
1	1A	1631	C	C2-N3-C4	5.56	122.68	119.90
1	1A	1889	A	N7-C8-N9	-5.56	111.02	113.80
1	1A	2539	C	N3-C4-C5	5.56	124.12	121.90
1	2A	1120	G	N1-C6-O6	5.56	123.24	119.90
1	2A	1430	C	C5-C6-N1	5.56	123.78	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2111	C	C2-N3-C4	5.56	122.68	119.90
1	1A	667	U	OP2-P-O3'	5.56	117.43	105.20
2	1B	64	C	O5'-P-OP2	-5.56	100.70	105.70
1	2A	646	A	N7-C8-N9	5.56	116.58	113.80
1	2A	678	C	C5-C6-N1	-5.56	118.22	121.00
1	2A	1683	C	OP2-P-O3'	5.56	117.42	105.20
1	1A	690	G	N7-C8-N9	-5.56	110.32	113.10
1	1A	1236	G	N7-C8-N9	-5.56	110.32	113.10
1	2A	2591	C	OP1-P-O3'	5.56	117.42	105.20
1	2A	2718	G	C5-N7-C8	-5.56	101.52	104.30
1	1A	750	A	C5-C6-N6	5.55	128.14	123.70
1	1A	1220	A	C4-C5-N7	-5.55	107.92	110.70
1	2A	301	G	C2-N3-C4	-5.55	109.12	111.90
1	2A	563	G	OP1-P-OP2	5.55	127.93	119.60
1	2A	808	G	C5-C6-N1	5.55	114.28	111.50
32	2a	829	G	N7-C8-N9	5.55	115.88	113.10
1	2A	932	G	C4-C5-N7	-5.55	108.58	110.80
1	2A	1626	G	N9-C4-C5	5.55	107.62	105.40
32	2a	125	U	N1-C2-N3	5.55	118.23	114.90
1	1A	197	A	N1-C2-N3	5.55	132.07	129.30
1	1A	252	G	N1-C6-O6	-5.55	116.57	119.90
1	1A	684	G	C8-N9-C4	-5.55	104.18	106.40
1	1A	1062	G	N9-C4-C5	-5.55	103.18	105.40
1	1A	1128	A	OP2-P-O3'	5.55	117.41	105.20
1	1A	1594	G	C5-C6-N1	-5.55	108.72	111.50
1	1A	2430	A	N1-C2-N3	5.55	132.08	129.30
2	1B	102	A	C5-C6-N1	5.55	120.48	117.70
32	1a	1304	G	N3-C4-C5	-5.55	125.82	128.60
1	2A	197	A	C6-N1-C2	-5.55	115.27	118.60
1	2A	233	A	C8-N9-C4	5.55	108.02	105.80
1	2A	452	G	C4-N9-C1'	5.55	133.72	126.50
1	2A	2501	C	C2-N1-C1'	-5.55	112.69	118.80
1	2A	2692	C	OP2-P-O3'	-5.55	92.99	105.20
1	2A	96	G	C4-C5-N7	5.55	113.02	110.80
1	2A	1981	A	N7-C8-N9	5.55	116.58	113.80
1	2A	2275	C	O4'-C1'-N1	-5.55	103.76	108.20
32	2a	391	G	N3-C4-C5	5.55	131.38	128.60
32	2a	402	G	N1-C6-O6	-5.55	116.57	119.90
1	1A	1092	C	C5-C6-N1	5.55	123.77	121.00
1	1A	1672	C	OP1-P-O3'	5.55	117.41	105.20
1	2A	1976	U	C2-N1-C1'	5.55	124.36	117.70
1	2A	2121	G	N3-C4-N9	5.55	129.33	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2372	G	C5-C6-N1	-5.55	108.73	111.50
1	2A	2820	A	O4'-C1'-N9	5.55	112.64	108.20
1	1A	734	A	C5-C6-N1	-5.55	114.93	117.70
1	1A	1066	U	C5-C6-N1	5.55	125.47	122.70
1	1A	1280	G	N3-C2-N2	-5.55	116.02	119.90
1	1A	1360	A	C8-N9-C4	5.55	108.02	105.80
1	2A	1554	A	N1-C6-N6	-5.55	115.27	118.60
1	1A	949	C	C4-C5-C6	5.54	120.17	117.40
1	1A	1830	C	C4-C5-C6	-5.54	114.63	117.40
1	2A	681	G	N1-C6-O6	5.54	123.23	119.90
1	1A	378	C	C2-N3-C4	-5.54	117.13	119.90
1	1A	1299	G	O5'-P-OP2	5.54	117.35	110.70
1	1A	2376	A	O5'-P-OP1	-5.54	100.71	105.70
1	1A	2680	C	C2-N3-C4	5.54	122.67	119.90
32	1a	728	A	N7-C8-N9	5.54	116.57	113.80
32	1a	1442	G	C8-N9-C1'	-5.54	119.79	127.00
1	2A	194	G	N3-C2-N2	-5.54	116.02	119.90
1	2A	711	G	C5-C6-N1	-5.54	108.73	111.50
1	1A	231	C	C4-C5-C6	5.54	120.17	117.40
1	1A	398	G	C5-N7-C8	5.54	107.07	104.30
1	1A	1431	U	N1-C2-N3	-5.54	111.58	114.90
1	1A	2032	G	C8-N9-C4	5.54	108.62	106.40
32	1a	879	C	C6-N1-C2	5.54	122.52	120.30
1	2A	1132	A	OP2-P-O3'	5.54	117.39	105.20
1	2A	2191	G	C5-C6-O6	-5.54	125.28	128.60
1	2A	2617	C	C4-C5-C6	5.54	120.17	117.40
1	2A	1981	A	C4-C5-N7	5.54	113.47	110.70
1	1A	261	G	C2-N3-C4	-5.54	109.13	111.90
1	1A	1924	C	C6-N1-C2	-5.54	118.08	120.30
1	1A	1992	G	N9-C4-C5	-5.54	103.18	105.40
1	1A	2115	G	C2-N3-C4	5.54	114.67	111.90
1	1A	2321	G	C8-N9-C4	-5.54	104.19	106.40
1	1A	2414	G	C2-N3-C4	-5.54	109.13	111.90
1	1A	2487	G	N3-C4-C5	5.54	131.37	128.60
2	1B	66	A	C2-N3-C4	5.54	113.37	110.60
32	1a	807	A	C8-N9-C4	-5.54	103.58	105.80
1	2A	416	C	C6-N1-C2	5.54	122.52	120.30
1	2A	2825	C	O5'-P-OP1	-5.54	100.72	105.70
32	2a	870	U	C6-N1-C2	5.54	124.32	121.00
1	1A	2705	A	C2-N3-C4	-5.54	107.83	110.60
1	2A	2508	G	C5-C6-O6	-5.54	125.28	128.60
1	1A	81	G	C4-C5-N7	5.54	113.01	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	201	C	C2-N3-C4	-5.54	117.13	119.90
1	1A	272(E)	G	N3-C4-C5	5.54	131.37	128.60
1	1A	383	U	N3-C4-C5	-5.54	111.28	114.60
1	1A	761	A	C8-N9-C4	5.54	108.01	105.80
1	1A	774	A	O5'-P-OP2	-5.54	100.72	105.70
1	1A	1601	G	C6-C5-N7	-5.54	127.08	130.40
1	1A	2081	C	C2-N3-C4	-5.54	117.13	119.90
1	1A	2262	U	OP1-P-OP2	-5.54	111.30	119.60
1	1A	2452	C	OP2-P-O3'	5.54	117.38	105.20
32	1a	66	G	C5-N7-C8	-5.54	101.53	104.30
1	2A	399	G	C6-C5-N7	-5.54	127.08	130.40
1	2A	507	A	C5-N7-C8	-5.54	101.13	103.90
1	2A	791	C	O4'-C1'-N1	5.54	112.63	108.20
1	2A	1674	G	OP1-P-O3'	5.54	117.38	105.20
1	2A	1678	G	N3-C4-C5	-5.54	125.83	128.60
1	2A	2163	C	C5-C6-N1	5.54	123.77	121.00
1	2A	2347	C	C6-N1-C2	-5.54	118.09	120.30
1	2A	2601	C	N3-C4-C5	5.54	124.11	121.90
1	1A	620	G	N1-C6-O6	5.53	123.22	119.90
1	1A	1187	G	O5'-P-OP2	-5.53	100.72	105.70
1	1A	1469	A	OP2-P-O3'	5.53	117.37	105.20
1	1A	2069	G	OP1-P-OP2	-5.53	111.30	119.60
32	1a	979	C	N3-C4-C5	-5.53	119.69	121.90
32	1a	1505	G	N1-C6-O6	-5.53	116.58	119.90
1	2A	1128	A	O5'-P-OP2	-5.53	100.72	105.70
1	2A	1525	G	O5'-P-OP2	-5.53	100.72	105.70
1	2A	1776	G	N1-C2-N3	5.53	127.22	123.90
1	2A	2032	G	N1-C2-N3	5.53	127.22	123.90
32	2a	1041	A	O4'-C1'-N9	5.53	112.63	108.20
32	2a	1419	G	O5'-P-OP1	5.53	117.34	110.70
1	1A	1221	C	OP1-P-O3'	5.53	117.37	105.20
32	1a	1437	C	O5'-P-OP1	-5.53	100.72	105.70
1	1A	834	C	OP2-P-O3'	5.53	117.36	105.20
1	1A	2220	G	C5-C6-N1	-5.53	108.73	111.50
1	1A	2684	U	C5-C6-N1	-5.53	119.93	122.70
1	2A	1188	U	N3-C2-O2	-5.53	118.33	122.20
32	2a	300	A	C5-C6-N6	-5.53	119.28	123.70
32	2a	1357	A	C8-N9-C4	-5.53	103.59	105.80
32	1a	284	G	N3-C2-N2	-5.53	116.03	119.90
32	2a	266	G	C8-N9-C4	-5.53	104.19	106.40
1	1A	525	U	OP1-P-OP2	5.53	127.89	119.60
1	1A	622	G	C5-C6-N1	-5.53	108.74	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	733	G	N1-C2-N2	-5.53	111.23	116.20
1	1A	762	U	N1-C2-N3	5.53	118.22	114.90
1	1A	965	C	N3-C2-O2	5.53	125.77	121.90
1	1A	1399	C	OP1-P-O3'	-5.53	93.04	105.20
1	1A	1601	G	C5-C6-O6	-5.53	125.28	128.60
1	1A	1784	A	C8-N9-C4	5.53	108.01	105.80
1	1A	1896	G	C5-C6-N1	-5.53	108.74	111.50
1	1A	1897	G	N9-C4-C5	-5.53	103.19	105.40
32	1a	830	G	N3-C4-C5	5.53	131.36	128.60
32	1a	892	A	N9-C4-C5	-5.53	103.59	105.80
1	2A	458	G	C8-N9-C4	-5.53	104.19	106.40
1	2A	1597	A	N7-C8-N9	-5.53	111.04	113.80
1	2A	1667	G	OP2-P-O3'	5.53	117.36	105.20
1	1A	475	U	C5-C6-N1	-5.53	119.94	122.70
1	1A	772	C	N3-C4-N4	5.53	121.87	118.00
1	1A	810	U	C5-C6-N1	5.53	125.46	122.70
1	1A	1021	A	C5-C6-N6	5.53	128.12	123.70
1	1A	1253	A	C5-N7-C8	5.53	106.66	103.90
1	1A	1986	A	C8-N9-C4	5.53	108.01	105.80
1	1A	2582	G	C5-N7-C8	-5.53	101.54	104.30
1	1A	2823	A	N7-C8-N9	5.53	116.56	113.80
32	1a	558	G	O5'-P-OP1	-5.53	100.73	105.70
32	1a	705	U	N1-C2-N3	5.53	118.22	114.90
1	2A	331	A	N7-C8-N9	5.53	116.56	113.80
1	2A	2286	A	C6-N1-C2	-5.53	115.28	118.60
1	2A	2302	G	N3-C4-C5	-5.53	125.84	128.60
32	2a	52	G	OP1-P-O3'	5.53	117.36	105.20
1	1A	1653	G	N1-C6-O6	5.52	123.21	119.90
1	2A	951	C	C5-C6-N1	5.52	123.76	121.00
1	1A	530	G	N1-C2-N3	-5.52	120.59	123.90
1	1A	1216	G	C4-C5-N7	-5.52	108.59	110.80
1	1A	2172	U	N3-C4-O4	-5.52	115.53	119.40
32	1a	127	G	N3-C2-N2	-5.52	116.03	119.90
32	1a	1397	C	C2-N3-C4	5.52	122.66	119.90
1	2A	98	G	C8-N9-C4	5.52	108.61	106.40
1	2A	197	A	C2-N3-C4	5.52	113.36	110.60
32	2a	117	G	N3-C4-N9	5.52	129.31	126.00
1	1A	1006	C	C4-C5-C6	5.52	120.16	117.40
1	1A	2764	A	C4-C5-N7	-5.52	107.94	110.70
1	1A	211	A	OP2-P-O3'	5.52	117.34	105.20
1	1A	228	A	N7-C8-N9	5.52	116.56	113.80
32	1a	1281	U	O5'-P-OP2	-5.52	100.73	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2518	A	O5'-P-OP2	5.52	117.32	110.70
1	2A	2824	C	N3-C4-C5	-5.52	119.69	121.90
32	2a	276	G	N1-C6-O6	-5.52	116.59	119.90
1	1A	478	A	OP2-P-O3'	5.52	117.34	105.20
1	1A	619	G	C8-N9-C4	5.52	108.61	106.40
1	1A	1368	G	C2-N3-C4	5.52	114.66	111.90
1	1A	2053	G	N3-C2-N2	-5.52	116.04	119.90
1	1A	2263	C	OP1-P-OP2	-5.52	111.32	119.60
32	1a	730	G	C4-C5-N7	-5.52	108.59	110.80
1	2A	1231	G	C2-N3-C4	-5.52	109.14	111.90
1	2A	1264	G	C4-C5-C6	5.52	122.11	118.80
1	2A	1547	C	N3-C4-C5	-5.52	119.69	121.90
1	2A	1552	G	N3-C4-C5	5.52	131.36	128.60
1	2A	1932	A	C5-C6-N6	-5.52	119.29	123.70
1	2A	2032	G	C4-N9-C1'	-5.52	119.33	126.50
1	2A	2562	U	C6-N1-C2	-5.52	117.69	121.00
2	2B	13	A	O5'-P-OP2	-5.52	100.73	105.70
32	2a	28	G	C5-C6-N1	-5.52	108.74	111.50
32	2a	508	C	C5-C4-N4	-5.52	116.34	120.20
1	1A	2114	A	N1-C6-N6	-5.52	115.29	118.60
1	2A	1707	G	C5-C6-N1	5.52	114.26	111.50
32	2a	898	G	C8-N9-C4	5.52	108.61	106.40
1	1A	818	G	N3-C2-N2	-5.51	116.04	119.90
1	1A	1901	A	O5'-P-OP2	-5.51	100.74	105.70
1	1A	2152	G	N9-C4-C5	-5.51	103.19	105.40
32	1a	755	G	N1-C6-O6	5.51	123.21	119.90
1	2A	450	G	C8-N9-C4	-5.51	104.19	106.40
1	2A	1558	A	C2-N3-C4	-5.51	107.84	110.60
32	2a	1416	G	C2-N3-C4	-5.51	109.14	111.90
1	1A	409	C	C6-N1-C2	5.51	122.50	120.30
32	1a	1501	C	N3-C2-O2	5.51	125.76	121.90
1	2A	2244	U	N1-C2-O2	-5.51	118.94	122.80
1	2A	2577	A	C5-N7-C8	-5.51	101.14	103.90
1	1A	447	A	N1-C6-N6	5.51	121.91	118.60
1	1A	2373	G	OP1-P-OP2	5.51	127.87	119.60
1	1A	2454	G	C4-C5-N7	-5.51	108.60	110.80
1	1A	2794	C	C6-N1-C2	-5.51	118.09	120.30
1	2A	988	A	C4-C5-N7	5.51	113.45	110.70
1	2A	1673	U	C6-N1-C2	5.51	124.31	121.00
1	2A	2018	G	N3-C4-C5	5.51	131.36	128.60
1	2A	2295	C	C5-C6-N1	5.51	123.76	121.00
32	2a	404	U	C5-C6-N1	5.51	125.46	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	548	G	N1-C6-O6	5.51	123.21	119.90
32	2a	802	A	N7-C8-N9	5.51	116.56	113.80
32	2a	970	C	C5-C6-N1	5.51	123.75	121.00
32	2a	1348	U	N3-C2-O2	-5.51	118.34	122.20
1	1A	904	C	C5-C4-N4	5.51	124.06	120.20
1	1A	913	U	C5-C6-N1	5.51	125.45	122.70
1	1A	1155	A	N7-C8-N9	-5.51	111.05	113.80
1	1A	1924	C	N1-C2-O2	-5.51	115.59	118.90
1	1A	1990	C	N1-C2-O2	-5.51	115.59	118.90
4	1E	164	ARG	NE-CZ-NH1	-5.51	117.55	120.30
32	1a	1121	U	C5-C6-N1	5.51	125.45	122.70
1	2A	1758	G	C5-C6-O6	-5.51	125.29	128.60
1	2A	2011	U	C5-C4-O4	-5.51	122.59	125.90
1	2A	2283	C	C6-N1-C2	5.51	122.50	120.30
1	2A	2832	U	C6-N1-C1'	-5.51	113.49	121.20
32	2a	584	G	C5-C6-N1	5.51	114.25	111.50
1	1A	2060	A	C8-N9-C4	-5.51	103.60	105.80
1	1A	2488	A	O5'-P-OP2	-5.51	100.74	105.70
1	2A	194	G	OP2-P-O3'	5.51	117.32	105.20
1	2A	1934	C	O5'-P-OP1	5.51	117.31	110.70
1	2A	2457	U	N3-C2-O2	-5.51	118.34	122.20
1	1A	623	G	C5-C6-N1	5.51	114.25	111.50
1	1A	1046	A	C2-N3-C4	5.51	113.35	110.60
1	1A	2266	A	O5'-P-OP1	-5.51	100.74	105.70
1	1A	2312	U	C5-C6-N1	5.51	125.45	122.70
1	1A	2693	A	OP1-P-OP2	-5.51	111.34	119.60
2	1B	104	U	C2-N3-C4	-5.51	123.70	127.00
32	1a	498	U	N3-C4-O4	-5.51	115.55	119.40
1	2A	402	A	C8-N9-C4	5.51	108.00	105.80
1	2A	795	C	N1-C2-O2	-5.51	115.60	118.90
1	2A	1047	G	N3-C4-N9	5.51	129.30	126.00
1	2A	1447	G	C8-N9-C4	-5.51	104.20	106.40
32	2a	226	G	C6-C5-N7	5.51	133.70	130.40
32	2a	1127	G	C8-N9-C4	5.51	108.60	106.40
32	2a	1442	G	P-O3'-C3'	5.51	126.31	119.70
1	1A	607	U	C6-N1-C2	5.50	124.30	121.00
1	1A	1756	G	C5-N7-C8	5.50	107.05	104.30
1	1A	1773	A	O5'-P-OP1	5.50	117.31	110.70
1	1A	2363	C	C6-N1-C2	5.50	122.50	120.30
1	2A	1425	G	O5'-P-OP2	-5.50	100.75	105.70
1	2A	2139	C	N1-C2-O2	5.50	122.20	118.90
1	2A	2473	U	C2-N1-C1'	5.50	124.31	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	998	C	C6-N1-C2	-5.50	118.10	120.30
1	1A	1295	C	C6-N1-C2	5.50	122.50	120.30
1	1A	1502	C	N1-C2-O2	-5.50	115.60	118.90
1	1A	1844	C	N3-C2-O2	5.50	125.75	121.90
1	1A	2487	G	C4-C5-N7	5.50	113.00	110.80
1	2A	521	G	C5-C6-N1	-5.50	108.75	111.50
1	1A	1096	A	C5-C6-N6	5.50	128.10	123.70
1	1A	1189	A	N9-C4-C5	-5.50	103.60	105.80
1	1A	1626	G	C2-N3-C4	-5.50	109.15	111.90
1	1A	2065	C	N3-C4-N4	-5.50	114.15	118.00
32	1a	318	G	N3-C2-N2	-5.50	116.05	119.90
1	2A	321	G	C8-N9-C4	5.50	108.60	106.40
1	2A	825	C	C4-C5-C6	5.50	120.15	117.40
1	2A	2047	U	O5'-P-OP2	-5.50	100.75	105.70
1	2A	1265	A	N9-C4-C5	-5.50	103.60	105.80
1	2A	2871	C	O5'-P-OP1	5.50	117.30	110.70
32	2a	481	G	C8-N9-C1'	-5.50	119.85	127.00
1	1A	208	C	N1-C2-O2	-5.50	115.60	118.90
1	1A	478	A	N7-C8-N9	5.50	116.55	113.80
1	1A	751	A	N3-C4-C5	-5.50	122.95	126.80
1	1A	775	G	N9-C4-C5	-5.50	103.20	105.40
1	1A	1841	U	C5-C4-O4	5.50	129.20	125.90
1	1A	1852	C	N1-C2-O2	-5.50	115.60	118.90
1	1A	2878	U	N1-C2-N3	5.50	118.20	114.90
32	1a	244	U	C6-N1-C2	5.50	124.30	121.00
1	2A	177	G	N3-C4-C5	5.50	131.35	128.60
1	2A	308	G	N3-C4-C5	5.50	131.35	128.60
1	2A	586	A	C8-N9-C4	5.50	108.00	105.80
1	2A	1785	A	C5-C6-N6	-5.50	119.30	123.70
1	2A	1883	G	C5-N7-C8	5.50	107.05	104.30
1	2A	2323	G	N3-C4-N9	-5.50	122.70	126.00
1	2A	2595	G	OP2-P-O3'	5.50	117.30	105.20
1	1A	1792	G	C6-C5-N7	5.50	133.70	130.40
1	1A	2465	C	C5-C4-N4	-5.50	116.35	120.20
1	1A	2471	C	C6-N1-C2	-5.50	118.10	120.30
1	1A	2767	C	N3-C4-C5	-5.50	119.70	121.90
1	1A	2819	G	N3-C4-C5	5.50	131.35	128.60
2	1B	51	G	C5-C6-O6	-5.50	125.30	128.60
1	2A	658	C	N1-C2-N3	5.50	123.05	119.20
1	2A	2148	G	C4-N9-C1'	-5.50	119.35	126.50
2	2B	53	A	O5'-P-OP1	-5.50	100.75	105.70
2	2B	85	G	OP1-P-OP2	5.50	127.84	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	380	G	C8-N9-C4	-5.50	104.20	106.40
32	2a	894	G	C5-C6-O6	-5.50	125.30	128.60
32	2a	1517	G	C8-N9-C4	5.50	108.60	106.40
1	1A	119	A	C6-N1-C2	-5.50	115.30	118.60
1	1A	1283	G	C5-C6-O6	5.50	131.90	128.60
1	1A	1938	A	N1-C2-N3	5.50	132.05	129.30
32	1a	244	U	C5-C4-O4	-5.50	122.60	125.90
1	2A	797	C	N3-C4-C5	-5.50	119.70	121.90
1	1A	411	G	C4-C5-N7	-5.49	108.60	110.80
1	1A	473	G	N7-C8-N9	-5.49	110.35	113.10
1	1A	686	G	C8-N9-C4	5.49	108.60	106.40
1	1A	2060	A	C5-C6-N6	5.49	128.09	123.70
1	1A	2447	G	C6-C5-N7	-5.49	127.10	130.40
1	2A	148	C	N3-C4-N4	5.49	121.84	118.00
1	2A	1654	A	N1-C6-N6	-5.49	115.30	118.60
1	2A	2062	A	C4-C5-N7	5.49	113.45	110.70
1	2A	2245	U	C5-C4-O4	-5.49	122.60	125.90
1	2A	2357	U	N3-C2-O2	-5.49	118.35	122.20
1	2A	2580	U	N3-C4-C5	-5.49	111.30	114.60
1	2A	2609	U	C5-C6-N1	-5.49	119.95	122.70
1	1A	2134	A	N1-C6-N6	-5.49	115.31	118.60
1	1A	2763	G	O5'-P-OP2	-5.49	100.76	105.70
32	2a	378	G	O5'-P-OP1	5.49	117.29	110.70
32	2a	511	C	OP2-P-O3'	5.49	117.28	105.20
1	1A	635	C	N3-C4-C5	-5.49	119.70	121.90
1	1A	681	G	C2-N3-C4	-5.49	109.16	111.90
1	1A	739	G	P-O5'-C5'	-5.49	112.11	120.90
1	1A	828	U	N3-C4-O4	5.49	123.24	119.40
1	1A	2144	U	C6-N1-C2	-5.49	117.70	121.00
1	1A	2335	A	C4-C5-N7	-5.49	107.95	110.70
1	2A	2508	G	N3-C4-N9	5.49	129.29	126.00
1	1A	1373	A	OP1-P-OP2	-5.49	111.37	119.60
1	1A	1486	A	O5'-P-OP1	5.49	117.29	110.70
10	1O	8	LEU	CA-CB-CG	5.49	127.92	115.30
32	1a	900	A	C8-N9-C4	5.49	108.00	105.80
1	2A	1319	G	O4'-C1'-N9	-5.49	103.81	108.20
1	2A	2705	A	N7-C8-N9	-5.49	111.06	113.80
16	2U	55	ARG	NE-CZ-NH1	-5.49	117.56	120.30
32	2a	280	C	C6-N1-C2	5.49	122.50	120.30
1	1A	593	G	C8-N9-C4	-5.49	104.20	106.40
1	1A	1125	G	C6-N1-C2	-5.49	121.81	125.10
1	2A	599	G	C2-N3-C4	-5.49	109.16	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1047	G	N1-C6-O6	-5.49	116.61	119.90
1	1A	1579	A	C5-C6-N6	-5.49	119.31	123.70
1	1A	2422	A	OP1-P-OP2	5.49	127.83	119.60
1	1A	2423	U	OP1-P-O3'	5.49	117.27	105.20
32	1a	1503	A	O5'-P-OP1	-5.49	100.76	105.70
1	2A	924	C	O5'-P-OP2	-5.49	100.76	105.70
1	2A	1159	U	C2-N3-C4	-5.49	123.71	127.00
1	2A	1721	G	C5-C6-N1	5.49	114.24	111.50
1	2A	1932	A	N9-C4-C5	-5.49	103.61	105.80
1	1A	1393	A	C5-C6-N1	5.48	120.44	117.70
1	1A	2766	G	C4-C5-N7	-5.48	108.61	110.80
1	2A	2778	A	O5'-P-OP2	-5.48	100.77	105.70
32	2a	910	C	OP1-P-OP2	-5.48	111.37	119.60
32	2a	1007	C	C5-C6-N1	5.48	123.74	121.00
1	1A	21	A	C4-C5-N7	5.48	113.44	110.70
1	1A	299	A	OP2-P-O3'	5.48	117.26	105.20
1	1A	766	C	C2-N3-C4	-5.48	117.16	119.90
1	1A	1029	A	O5'-P-OP1	5.48	117.28	110.70
1	1A	1256	G	C4-N9-C1'	5.48	133.63	126.50
1	1A	2238	G	N3-C4-C5	-5.48	125.86	128.60
1	1A	2398	U	C5-C6-N1	-5.48	119.96	122.70
1	2A	1512	U	N1-C2-O2	-5.48	118.96	122.80
1	2A	2599	G	C2-N3-C4	-5.48	109.16	111.90
1	2A	2840	C	O5'-P-OP2	-5.48	100.77	105.70
32	2a	299	G	C5-C6-N1	5.48	114.24	111.50
32	2a	550	G	N3-C4-C5	5.48	131.34	128.60
32	2a	980	C	N1-C2-O2	5.48	122.19	118.90
1	1A	1192	G	OP2-P-O3'	5.48	117.25	105.20
1	1A	1300	U	C5-C4-O4	5.48	129.19	125.90
1	1A	1568	G	C4-C5-C6	5.48	122.09	118.80
32	1a	698	G	C8-N9-C4	-5.48	104.21	106.40
1	2A	100	G	N3-C4-C5	-5.48	125.86	128.60
1	2A	413	C	C6-N1-C2	5.48	122.49	120.30
1	2A	721	C	C6-N1-C2	5.48	122.49	120.30
1	2A	1287	A	C4-C5-N7	5.48	113.44	110.70
32	2a	1027	C	N3-C4-C5	-5.48	119.71	121.90
42	2k	63	LEU	CA-CB-CG	5.48	127.91	115.30
1	1A	2535	G	C4-N9-C1'	-5.48	119.38	126.50
1	2A	1660	C	C6-N1-C1'	5.48	127.38	120.80
32	2a	1112	C	C6-N1-C2	-5.48	118.11	120.30
1	1A	81	G	N9-C4-C5	-5.48	103.21	105.40
1	1A	205	G	C8-N9-C4	5.48	108.59	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	250	G	N9-C4-C5	5.48	107.59	105.40
1	1A	906	G	C6-N1-C2	5.48	128.39	125.10
1	1A	1008	C	C6-N1-C1'	-5.48	114.23	120.80
1	1A	1152	C	N3-C4-C5	5.48	124.09	121.90
1	1A	1252	G	N9-C4-C5	5.48	107.59	105.40
1	1A	1997	G	N9-C4-C5	5.48	107.59	105.40
1	1A	2259	G	C6-C5-N7	-5.48	127.11	130.40
1	1A	2329	G	O5'-P-OP1	-5.48	100.77	105.70
1	1A	2485	G	N1-C6-O6	5.48	123.19	119.90
1	1A	2573	C	C2-N1-C1'	5.48	124.83	118.80
1	2A	69	C	O5'-P-OP2	-5.48	100.77	105.70
1	1A	940	G	N7-C8-N9	5.48	115.84	113.10
32	1a	376	G	N3-C4-C5	5.48	131.34	128.60
1	2A	696	G	C5-C6-N1	-5.48	108.76	111.50
1	2A	1820	U	N3-C4-C5	5.48	117.89	114.60
1	2A	1905	C	C6-N1-C2	-5.48	118.11	120.30
1	2A	2387	U	C6-N1-C2	5.48	124.28	121.00
1	2A	2526	G	C5-C6-N1	-5.48	108.76	111.50
32	2a	1456	G	N3-C4-C5	5.48	131.34	128.60
1	1A	1812	A	O5'-P-OP1	-5.47	100.77	105.70
1	1A	2578	G	C4-C5-N7	-5.47	108.61	110.80
1	2A	446	G	N9-C4-C5	-5.47	103.21	105.40
1	2A	2526	G	C6-C5-N7	-5.47	127.11	130.40
1	1A	596	G	C8-N9-C4	5.47	108.59	106.40
1	1A	1239	G	C4-C5-C6	5.47	122.08	118.80
1	2A	535	C	OP2-P-O3'	5.47	117.24	105.20
1	2A	1286	A	N9-C4-C5	5.47	107.99	105.80
32	2a	1348	U	C6-N1-C2	-5.47	117.72	121.00
1	1A	135	G	N9-C1'-C2'	-5.47	105.98	112.00
1	1A	1414	G	N1-C6-O6	5.47	123.18	119.90
1	1A	1815	A	N1-C6-N6	-5.47	115.32	118.60
13	1R	51	LEU	CB-CG-CD1	-5.47	101.70	111.00
1	2A	1260	G	N7-C8-N9	-5.47	110.36	113.10
32	2a	803	G	N1-C2-N3	5.47	127.18	123.90
1	1A	673	C	O5'-P-OP2	-5.47	100.78	105.70
1	1A	739	G	C2-N3-C4	-5.47	109.17	111.90
32	1a	35	G	N7-C8-N9	5.47	115.83	113.10
32	1a	1067	A	O4'-C1'-N9	-5.47	103.83	108.20
1	2A	794	G	C2-N3-C4	-5.47	109.17	111.90
1	2A	2603	G	C4-C5-N7	-5.47	108.61	110.80
1	1A	641	C	C5-C6-N1	5.47	123.73	121.00
1	1A	829	A	N9-C4-C5	-5.47	103.61	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1633	G	C5-C6-N1	5.47	114.23	111.50
1	2A	1604	C	N1-C2-O2	-5.47	115.62	118.90
1	2A	2827	C	N3-C2-O2	5.47	125.73	121.90
1	1A	99	U	O4'-C1'-N1	5.47	112.57	108.20
1	1A	104	U	OP2-P-O3'	5.47	117.22	105.20
1	1A	769	G	OP2-P-O3'	5.47	117.23	105.20
1	1A	2244	U	N1-C2-O2	-5.47	118.97	122.80
1	1A	2685	G	N3-C4-N9	-5.47	122.72	126.00
2	1B	98	G	OP1-P-OP2	5.47	127.80	119.60
1	2A	217	G	N3-C2-N2	5.47	123.73	119.90
1	2A	899	A	N9-C4-C5	5.47	107.99	105.80
1	2A	1860	G	N3-C4-C5	5.47	131.33	128.60
1	2A	2705	A	N9-C4-C5	-5.47	103.61	105.80
2	2B	24	G	C5-C6-N1	5.47	114.23	111.50
1	1A	1339	G	N1-C2-N3	5.46	127.18	123.90
1	1A	1792	G	C5-C6-O6	5.46	131.88	128.60
1	1A	2252	G	O5'-P-OP2	-5.46	100.78	105.70
32	1a	161	A	C8-N9-C4	-5.46	103.61	105.80
1	2A	63	U	N1-C2-O2	-5.46	118.97	122.80
1	2A	800	A	C5-C6-N1	-5.46	114.97	117.70
1	2A	1382	G	C5-C6-O6	-5.46	125.32	128.60
32	2a	230	G	C4-C5-C6	5.46	122.08	118.80
1	2A	1005	C	OP1-P-OP2	5.46	127.79	119.60
1	2A	1472	A	C5-C6-N6	-5.46	119.33	123.70
2	2B	61	G	OP1-P-OP2	5.46	127.80	119.60
1	1A	941	A	C2-N3-C4	5.46	113.33	110.60
1	1A	1026	U	C2-N1-C1'	5.46	124.25	117.70
1	1A	1646	C	N1-C2-O2	5.46	122.18	118.90
1	1A	1663	C	N1-C2-O2	-5.46	115.62	118.90
1	1A	1721	G	C5-C6-O6	-5.46	125.32	128.60
1	1A	1819	A	C2-N3-C4	-5.46	107.87	110.60
1	1A	2040	C	C5-C4-N4	-5.46	116.38	120.20
1	1A	2690	C	N3-C4-C5	-5.46	119.72	121.90
1	2A	10	G	N1-C2-N3	-5.46	120.62	123.90
1	2A	1392	A	C5-C6-N1	5.46	120.43	117.70
1	2A	1745	C	N3-C2-O2	5.46	125.72	121.90
1	2A	1847	A	N1-C6-N6	-5.46	115.32	118.60
1	2A	2857	G	O5'-P-OP1	-5.46	100.78	105.70
32	2a	264	U	N3-C4-O4	5.46	123.22	119.40
32	2a	706	A	C8-N9-C4	-5.46	103.62	105.80
32	2a	868	C	C5-C6-N1	-5.46	118.27	121.00
1	1A	2036	C	C6-N1-C1'	5.46	127.35	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2439	A	O4'-C1'-N9	-5.46	103.83	108.20
1	2A	1169	G	C5-C6-N1	-5.46	108.77	111.50
1	2A	1605	C	C6-N1-C2	-5.46	118.12	120.30
1	1A	748	G	OP2-P-O3'	-5.46	93.19	105.20
18	1W	82	LEU	CA-CB-CG	-5.46	102.74	115.30
1	2A	924	C	C2-N1-C1'	-5.46	112.80	118.80
1	2A	1964	G	C8-N9-C4	5.46	108.58	106.40
32	2a	1224	G	C8-N9-C4	-5.46	104.22	106.40
1	1A	25	U	N3-C2-O2	5.46	126.02	122.20
1	1A	28	A	C6-C5-N7	-5.46	128.48	132.30
1	1A	41	C	C5-C6-N1	-5.46	118.27	121.00
1	1A	1154	G	N1-C2-N3	5.46	127.17	123.90
1	1A	1618	A	N9-C4-C5	-5.46	103.62	105.80
1	1A	1930	G	OP1-P-OP2	5.46	127.78	119.60
32	1a	162	A	N7-C8-N9	5.46	116.53	113.80
32	1a	346	G	C5-C6-O6	-5.46	125.33	128.60
1	2A	438	G	N1-C2-N3	5.46	127.17	123.90
1	2A	1381	G	OP1-P-O3'	-5.46	93.20	105.20
1	2A	2390	U	N1-C2-O2	5.46	126.62	122.80
1	2A	2443	C	C4-C5-C6	5.46	120.13	117.40
2	2B	27	C	N1-C2-O2	5.46	122.17	118.90
32	2a	926	G	C4-N9-C1'	5.46	133.59	126.50
1	1A	85	G	OP1-P-OP2	5.46	127.78	119.60
1	1A	203	C	N1-C2-O2	-5.46	115.63	118.90
1	1A	953	A	C6-N1-C2	-5.46	115.33	118.60
1	1A	1192	G	N7-C8-N9	-5.46	110.37	113.10
1	1A	2361	A	C8-N9-C4	5.46	107.98	105.80
32	2a	1504	G	C8-N9-C4	5.46	108.58	106.40
1	1A	141	A	N1-C6-N6	5.45	121.87	118.60
1	1A	371	A	N9-C4-C5	-5.45	103.62	105.80
1	1A	677	A	N1-C2-N3	5.45	132.03	129.30
32	1a	911	U	C6-N1-C2	-5.45	117.73	121.00
1	2A	657	U	C6-N1-C2	5.45	124.27	121.00
1	2A	1853	A	C8-N9-C4	5.45	107.98	105.80
1	2A	2565	A	O5'-P-OP2	5.45	117.25	110.70
32	2a	498	U	C5-C4-O4	5.45	129.17	125.90
1	1A	2453	A	C2-N3-C4	5.45	113.33	110.60
1	1A	813	U	N1-C2-N3	5.45	118.17	114.90
1	1A	1025	G	C4-C5-N7	-5.45	108.62	110.80
1	1A	2010	G	N1-C6-O6	5.45	123.17	119.90
2	1B	106	G	C5-C6-O6	-5.45	125.33	128.60
32	1a	1151	A	N1-C6-N6	-5.45	115.33	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	356	G	C8-N9-C4	-5.45	104.22	106.40
1	2A	463	G	N3-C4-N9	-5.45	122.73	126.00
1	2A	2235	G	C2-N3-C4	-5.45	109.17	111.90
1	2A	2540	C	N3-C4-C5	5.45	124.08	121.90
1	2A	2657	A	O5'-P-OP1	-5.45	100.80	105.70
2	2B	75	G	C5-C6-N1	-5.45	108.78	111.50
1	1A	1131	G	C8-N9-C4	5.45	108.58	106.40
32	1a	657	G	N1-C2-N2	5.45	121.10	116.20
32	1a	681	C	C5-C6-N1	5.45	123.72	121.00
32	1a	740	U	OP1-P-OP2	5.45	127.77	119.60
1	2A	80	G	N9-C4-C5	5.45	107.58	105.40
1	2A	256	A	C5-C6-N1	-5.45	114.98	117.70
1	2A	720	C	C5-C6-N1	-5.45	118.28	121.00
32	2a	544	G	N3-C4-C5	5.45	131.32	128.60
1	1A	210	C	N1-C2-O2	-5.45	115.63	118.90
1	1A	1332	G	N1-C2-N2	-5.45	111.30	116.20
1	1A	1524	G	C5-C6-N1	-5.45	108.78	111.50
1	1A	2514	U	N3-C2-O2	5.45	126.01	122.20
1	2A	141	A	C5-C6-N6	-5.45	119.34	123.70
1	2A	329	G	N7-C8-N9	5.45	115.82	113.10
1	2A	494	G	C4-C5-N7	-5.45	108.62	110.80
1	2A	1065	U	C2-N1-C1'	-5.45	111.16	117.70
1	2A	1635	G	C8-N9-C4	5.45	108.58	106.40
1	2A	1838	C	N3-C2-O2	-5.45	118.09	121.90
1	2A	1926	U	O5'-P-OP2	-5.45	100.80	105.70
1	2A	1948	G	C5-C6-O6	5.45	131.87	128.60
2	2B	74	U	C5-C6-N1	-5.45	119.98	122.70
1	1A	122	G	N3-C2-N2	-5.45	116.09	119.90
1	1A	648	G	N1-C2-N3	5.45	127.17	123.90
1	1A	2859	G	N9-C4-C5	-5.45	103.22	105.40
32	1a	1391	U	N1-C2-N3	5.45	118.17	114.90
1	2A	453	C	O5'-P-OP2	5.45	117.23	110.70
1	2A	729	G	N1-C2-N2	5.45	121.10	116.20
1	2A	959	A	N7-C8-N9	5.45	116.52	113.80
1	2A	1866	C	C6-N1-C1'	-5.45	114.27	120.80
1	1A	105	C	C6-N1-C2	5.44	122.48	120.30
1	1A	383	U	C2-N3-C4	5.44	130.27	127.00
1	1A	2881	C	C6-N1-C2	-5.44	118.12	120.30
18	1W	10	VAL	CB-CA-C	-5.44	101.06	111.40
32	1a	1417	G	N3-C2-N2	5.44	123.71	119.90
1	2A	613	G	N1-C6-O6	5.44	123.17	119.90
1	2A	740	U	OP1-P-OP2	5.44	127.77	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2B	111	G	C4-N9-C1'	-5.44	119.42	126.50
1	1A	177	G	C8-N9-C4	-5.44	104.22	106.40
1	1A	399	G	C8-N9-C4	5.44	108.58	106.40
1	1A	920	G	N1-C6-O6	5.44	123.17	119.90
1	1A	2103	C	C2-N3-C4	5.44	122.62	119.90
1	1A	2162	G	N3-C4-N9	5.44	129.27	126.00
1	1A	2561	A	C6-N1-C2	-5.44	115.33	118.60
1	1A	2647	U	C5-C4-O4	5.44	129.17	125.90
1	1A	2705	A	C5-C6-N1	-5.44	114.98	117.70
32	1a	499	A	OP1-P-O3'	5.44	117.17	105.20
1	2A	575	A	O5'-P-OP1	-5.44	100.80	105.70
1	2A	792	G	C2-N3-C4	5.44	114.62	111.90
1	2A	1259	G	C2-N3-C4	-5.44	109.18	111.90
32	2a	353	A	C5-N7-C8	-5.44	101.18	103.90
32	2a	781	A	N1-C6-N6	-5.44	115.33	118.60
1	1A	579	G	C6-C5-N7	-5.44	127.14	130.40
1	1A	855	G	C4-C5-N7	5.44	112.98	110.80
1	1A	1323	U	OP1-P-O3'	5.44	117.17	105.20
1	1A	1650	G	OP1-P-OP2	-5.44	111.44	119.60
32	1a	576	G	N1-C2-N2	-5.44	111.30	116.20
32	1a	725	G	C5-C6-O6	-5.44	125.33	128.60
32	1a	1521	G	N9-C4-C5	-5.44	103.22	105.40
1	2A	599	G	N1-C2-N3	5.44	127.16	123.90
1	2A	678	C	OP1-P-O3'	5.44	117.17	105.20
1	1A	652(S)	C	C2-N3-C4	5.44	122.62	119.90
1	1A	1049	C	O5'-P-OP2	-5.44	100.81	105.70
1	1A	1683	C	N1-C2-N3	5.44	123.01	119.20
1	1A	2513	G	N1-C6-O6	5.44	123.16	119.90
1	1A	1783	A	N1-C6-N6	-5.44	115.34	118.60
1	1A	2561	A	C5-N7-C8	5.44	106.62	103.90
32	1a	189(G)	G	N3-C4-N9	-5.44	122.74	126.00
1	2A	346	A	C4-C5-N7	5.44	113.42	110.70
1	2A	2032	G	O4'-C1'-N9	-5.44	103.85	108.20
1	2A	2182	G	N3-C4-N9	-5.44	122.74	126.00
1	2A	2604	U	N3-C2-O2	-5.44	118.39	122.20
32	2a	172	A	N9-C4-C5	5.44	107.97	105.80
32	2a	1397	C	C2-N3-C4	5.44	122.62	119.90
1	1A	1046	A	N7-C8-N9	5.44	116.52	113.80
32	1a	1523	G	C2-N3-C4	5.44	114.62	111.90
1	2A	903	C	C6-N1-C2	5.44	122.47	120.30
1	1A	242	G	N3-C4-C5	5.43	131.32	128.60
1	1A	842	G	O5'-P-OP1	5.43	117.22	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1673	U	P-O3'-C3'	5.43	126.22	119.70
1	1A	2050	C	N3-C4-N4	5.43	121.81	118.00
1	1A	2224	G	N7-C8-N9	-5.43	110.38	113.10
1	2A	622	G	C5-C6-N1	-5.43	108.78	111.50
1	2A	2637	U	N3-C2-O2	5.43	126.00	122.20
32	2a	926	G	N3-C2-N2	5.43	123.70	119.90
32	2a	1204	A	C8-N9-C4	-5.43	103.63	105.80
1	1A	271	A	N9-C4-C5	-5.43	103.63	105.80
1	1A	481	G	C8-N9-C4	-5.43	104.23	106.40
1	1A	693	C	C5-C6-N1	-5.43	118.28	121.00
1	1A	1802	A	C5-N7-C8	-5.43	101.18	103.90
1	1A	2386	C	N1-C2-O2	5.43	122.16	118.90
32	1a	1030(A)	G	C8-N9-C4	-5.43	104.23	106.40
1	2A	2267	A	C8-N9-C1'	-5.43	117.92	127.70
1	1A	506	G	OP1-P-OP2	5.43	127.75	119.60
1	1A	602	G	C8-N9-C4	5.43	108.57	106.40
1	1A	695	G	OP1-P-OP2	-5.43	111.45	119.60
1	1A	2025	C	N3-C4-C5	-5.43	119.73	121.90
1	1A	2392	A	C2-N3-C4	-5.43	107.89	110.60
32	1a	498	U	C2-N1-C1'	5.43	124.22	117.70
1	2A	616	G	N7-C8-N9	-5.43	110.38	113.10
1	2A	1120	G	N9-C4-C5	-5.43	103.23	105.40
1	2A	1359	A	N9-C4-C5	-5.43	103.63	105.80
1	1A	1319	G	C5-N7-C8	-5.43	101.58	104.30
1	1A	1398	C	OP2-P-O3'	5.43	117.14	105.20
1	1A	2587	A	N1-C2-N3	5.43	132.01	129.30
1	2A	380	U	O5'-P-OP2	-5.43	100.81	105.70
1	2A	502	A	N7-C8-N9	-5.43	111.09	113.80
1	2A	767	U	O5'-P-OP2	-5.43	100.81	105.70
32	2a	168	G	N3-C4-N9	5.43	129.26	126.00
32	2a	884	U	O5'-P-OP2	-5.43	100.81	105.70
1	1A	298	G	O5'-P-OP2	-5.43	100.81	105.70
1	1A	659	C	N3-C4-C5	5.43	124.07	121.90
32	2a	528	C	C5-C6-N1	5.43	123.71	121.00
1	1A	41	C	C6-N1-C2	5.43	122.47	120.30
1	1A	1380	G	N3-C4-N9	5.43	129.26	126.00
1	1A	2514	U	C5-C6-N1	-5.43	119.99	122.70
1	2A	1653	G	C4-C5-C6	5.43	122.06	118.80
1	2A	1883	G	N3-C4-C5	-5.43	125.89	128.60
1	1A	522	G	C5-N7-C8	-5.42	101.59	104.30
1	1A	569	U	N3-C4-C5	5.42	117.85	114.60
1	1A	2772	C	N3-C4-N4	-5.42	114.20	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	473	G	C8-N9-C4	-5.42	104.23	106.40
32	2a	345	C	C5-C6-N1	5.42	123.71	121.00
32	2a	903	G	C5-C6-O6	-5.42	125.34	128.60
32	2a	1022	G	N9-C4-C5	-5.42	103.23	105.40
1	1A	338	G	N1-C6-O6	-5.42	116.65	119.90
1	1A	732	C	C6-N1-C2	-5.42	118.13	120.30
32	1a	531	U	C6-N1-C2	-5.42	117.75	121.00
1	2A	1604	C	N3-C4-C5	-5.42	119.73	121.90
1	1A	48	G	N3-C2-N2	-5.42	116.11	119.90
1	1A	845	G	O4'-C1'-N9	5.42	112.54	108.20
1	1A	1031	G	N1-C6-O6	5.42	123.15	119.90
1	1A	1215	G	N3-C4-N9	5.42	129.25	126.00
1	1A	1445(A)	C	C6-N1-C2	-5.42	118.13	120.30
1	2A	2084	C	C2-N1-C1'	-5.42	112.84	118.80
1	2A	2218	U	N1-C2-O2	5.42	126.59	122.80
3	2D	54	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	1A	500	G	C4-C5-N7	-5.42	108.63	110.80
1	1A	1122	G	C5-C6-O6	-5.42	125.35	128.60
1	1A	2157	G	C2-N3-C4	5.42	114.61	111.90
1	2A	655	A	C6-C5-N7	-5.42	128.51	132.30
1	2A	1287	A	C5-C6-N6	-5.42	119.36	123.70
1	2A	1479	G	C5-C6-O6	-5.42	125.35	128.60
1	1A	202	U	C4-C5-C6	5.42	122.95	119.70
1	1A	377	C	OP1-P-OP2	-5.42	111.47	119.60
1	1A	447	A	C5-N7-C8	-5.42	101.19	103.90
1	1A	861	A	N1-C6-N6	5.42	121.85	118.60
1	1A	1643	G	N3-C4-C5	-5.42	125.89	128.60
1	1A	2259	G	C4-C5-N7	5.42	112.97	110.80
1	1A	2588	G	N9-C4-C5	5.42	107.57	105.40
1	1A	2742	C	C4-C5-C6	5.42	120.11	117.40
1	2A	666	G	N1-C6-O6	5.42	123.15	119.90
1	2A	1661	G	O5'-P-OP2	-5.42	100.82	105.70
1	2A	2415	G	C4-C5-C6	5.42	122.05	118.80
32	2a	903	G	O5'-P-OP1	5.42	117.20	110.70
1	1A	867	C	N3-C2-O2	5.42	125.69	121.90
32	1a	259	G	C5-C6-O6	-5.42	125.35	128.60
32	1a	1266	G	C5-C6-N1	-5.42	108.79	111.50
1	2A	271(X)	G	O5'-P-OP1	-5.42	100.83	105.70
1	2A	839	U	N3-C4-O4	-5.42	115.61	119.40
1	2A	1259	G	N1-C2-N3	5.42	127.15	123.90
32	2a	776	G	N1-C2-N3	5.42	127.15	123.90
1	1A	1847	A	N3-C4-C5	-5.42	123.01	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1088	A	N9-C4-C5	-5.42	103.63	105.80
1	2A	1318	C	N1-C2-O2	-5.42	115.65	118.90
32	2a	1008	C	N3-C4-N4	-5.42	114.21	118.00
1	1A	486	C	C6-N1-C2	5.41	122.47	120.30
1	1A	2659	G	N3-C4-N9	-5.41	122.75	126.00
1	1A	2679	A	N7-C8-N9	-5.41	111.09	113.80
32	1a	506	G	O5'-P-OP2	5.41	117.20	110.70
32	1a	855	G	O5'-P-OP1	-5.41	100.83	105.70
32	1a	893	C	N1-C2-N3	-5.41	115.41	119.20
1	2A	592	G	N1-C6-O6	-5.41	116.65	119.90
1	2A	1006	C	OP1-P-O3'	5.41	117.11	105.20
1	2A	1498	C	C2-N3-C4	5.41	122.61	119.90
1	2A	1890	A	C5-N7-C8	5.41	106.61	103.90
1	2A	2284	C	C5-C6-N1	-5.41	118.29	121.00
1	2A	2622	C	C6-N1-C2	5.41	122.47	120.30
1	2A	2821	A	N3-C4-C5	5.41	130.59	126.80
32	2a	378	G	O5'-P-OP2	-5.41	100.83	105.70
1	1A	993	G	C4-C5-C6	-5.41	115.55	118.80
1	1A	1145	C	C5-C6-N1	5.41	123.71	121.00
1	1A	2340	G	O5'-P-OP2	-5.41	100.83	105.70
1	1A	2562	U	N1-C2-O2	-5.41	119.01	122.80
1	1A	2894	G	N3-C4-N9	-5.41	122.75	126.00
1	2A	184	C	C6-N1-C2	5.41	122.46	120.30
1	2A	201	C	C5-C6-N1	-5.41	118.30	121.00
1	2A	521	G	C2-N3-C4	-5.41	109.19	111.90
1	2A	2437	U	N1-C2-O2	-5.41	119.01	122.80
1	1A	865	C	C2-N3-C4	5.41	122.60	119.90
1	1A	2019	A	C4-C5-C6	5.41	119.70	117.00
1	1A	2495	G	N3-C2-N2	-5.41	116.11	119.90
1	1A	2637	U	N3-C2-O2	5.41	125.99	122.20
1	1A	2714	G	C4-C5-N7	5.41	112.96	110.80
2	1B	118	G	C6-N1-C2	5.41	128.34	125.10
32	1a	1300	G	C8-N9-C4	5.41	108.56	106.40
1	2A	652(S)	C	C5-C6-N1	5.41	123.70	121.00
1	2A	1679	U	C5-C6-N1	-5.41	120.00	122.70
32	2a	768	A	C5-C6-N1	-5.41	115.00	117.70
1	2A	1328	G	N3-C4-N9	5.41	129.24	126.00
2	2B	15	A	N7-C8-N9	-5.41	111.10	113.80
1	1A	116	C	C4-C5-C6	5.41	120.10	117.40
1	1A	804	A	N1-C6-N6	5.41	121.84	118.60
1	1A	1004	C	N3-C2-O2	-5.41	118.12	121.90
1	1A	2429	G	C2-N3-C4	5.41	114.60	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1F	104	LYS	CD-CE-NZ	5.41	124.13	111.70
32	1a	6	G	N3-C4-C5	-5.41	125.90	128.60
1	2A	1225	G	N1-C6-O6	-5.41	116.66	119.90
1	2A	1667	G	N3-C4-C5	5.41	131.30	128.60
1	2A	1926	U	O4'-C1'-N1	5.41	112.53	108.20
32	2a	791	G	C5-C6-N1	-5.41	108.80	111.50
1	1A	1252	G	C8-N9-C1'	5.40	134.03	127.00
22	10	77	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	2A	139(A)	G	C8-N9-C4	5.40	108.56	106.40
1	2A	1838	C	O4'-C1'-N1	5.40	112.52	108.20
1	2A	1935	G	C5-C6-N1	5.40	114.20	111.50
1	2A	2749	A	C8-N9-C4	5.40	107.96	105.80
32	2a	1522	U	N3-C4-C5	-5.40	111.36	114.60
1	1A	38	A	N3-C4-C5	-5.40	123.02	126.80
1	1A	1532	C	C6-N1-C2	-5.40	118.14	120.30
1	1A	2031	A	C8-N9-C4	-5.40	103.64	105.80
1	1A	2390	U	OP1-P-O3'	5.40	117.09	105.20
1	2A	1318	C	C6-N1-C2	-5.40	118.14	120.30
1	2A	1565	C	N3-C4-C5	5.40	124.06	121.90
32	2a	481	G	C4-C5-C6	5.40	122.04	118.80
32	2a	761	G	N3-C4-N9	-5.40	122.76	126.00
1	1A	118	A	N7-C8-N9	-5.40	111.10	113.80
1	1A	596	G	OP1-P-OP2	5.40	127.70	119.60
1	1A	726	G	C5-C6-N1	-5.40	108.80	111.50
1	1A	2070	G	N1-C2-N3	5.40	127.14	123.90
2	1B	39	A	C2-N3-C4	5.40	113.30	110.60
1	2A	80	G	C4-C5-N7	-5.40	108.64	110.80
1	2A	1791	A	OP1-P-OP2	-5.40	111.50	119.60
1	2A	1959	G	C5-C6-O6	5.40	131.84	128.60
32	2a	1146	A	C8-N9-C4	5.40	107.96	105.80
35	2d	135	LEU	CA-CB-CG	5.40	127.72	115.30
1	1A	136	G	N7-C8-N9	-5.40	110.40	113.10
1	1A	434	U	N1-C2-N3	5.40	118.14	114.90
1	1A	715	G	N3-C2-N2	5.40	123.68	119.90
1	1A	1003	G	N3-C4-N9	5.40	129.24	126.00
1	1A	1184	G	C5-C6-N1	-5.40	108.80	111.50
1	1A	1394	U	C6-N1-C2	-5.40	117.76	121.00
1	1A	1831	G	N7-C8-N9	5.40	115.80	113.10
1	1A	2645	G	N3-C4-C5	5.40	131.30	128.60
32	1a	803	G	N1-C6-O6	5.40	123.14	119.90
1	2A	729	G	N3-C2-N2	-5.40	116.12	119.90
1	1A	199	A	N1-C6-N6	-5.40	115.36	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	770	G	N1-C2-N3	5.40	127.14	123.90
1	1A	953	A	N1-C6-N6	-5.40	115.36	118.60
1	1A	1192	G	N1-C2-N3	5.40	127.14	123.90
1	1A	1394	U	N1-C2-O2	5.40	126.58	122.80
1	1A	1903	G	N9-C4-C5	-5.40	103.24	105.40
1	1A	1972	A	N1-C6-N6	5.40	121.84	118.60
1	1A	2437	U	N3-C4-C5	-5.40	111.36	114.60
1	1A	2701	C	N3-C2-O2	-5.40	118.12	121.90
32	1a	586	C	C2-N1-C1'	-5.40	112.86	118.80
1	2A	114	U	N1-C2-O2	-5.40	119.02	122.80
1	2A	1767	C	N3-C4-N4	-5.40	114.22	118.00
1	2A	2446	G	C2-N3-C4	-5.40	109.20	111.90
1	2A	2538	C	N1-C2-O2	5.40	122.14	118.90
32	2a	1500	A	N9-C4-C5	-5.40	103.64	105.80
1	1A	374	A	N1-C6-N6	5.40	121.84	118.60
1	1A	551	G	C5-C6-O6	-5.40	125.36	128.60
1	1A	730	C	N3-C4-C5	5.40	124.06	121.90
1	1A	832	G	N1-C2-N3	5.40	127.14	123.90
1	1A	1967	C	C6-N1-C2	-5.40	118.14	120.30
1	1A	2489	G	N1-C2-N2	-5.40	111.34	116.20
1	1A	2872	G	C2-N3-C4	-5.40	109.20	111.90
1	2A	390	A	C5-C6-N1	-5.40	115.00	117.70
1	1A	568	U	C6-N1-C2	5.39	124.24	121.00
1	1A	1099	G	N9-C4-C5	-5.39	103.24	105.40
1	1A	1365	A	OP1-P-OP2	5.39	127.69	119.60
1	1A	1762	A	C4-N9-C1'	-5.39	116.59	126.30
1	1A	1817	G	N3-C4-C5	-5.39	125.90	128.60
1	1A	2515	C	N3-C2-O2	5.39	125.68	121.90
1	1A	2701	C	N1-C2-N3	5.39	122.98	119.20
2	1B	75	G	C8-N9-C4	5.39	108.56	106.40
32	1a	435	C	C5-C6-N1	5.39	123.70	121.00
32	1a	722	A	C6-C5-N7	-5.39	128.52	132.30
32	1a	867	G	O5'-P-OP2	-5.39	100.85	105.70
1	2A	517	C	N3-C4-N4	5.39	121.78	118.00
1	2A	590	A	N1-C6-N6	5.39	121.84	118.60
1	2A	859	G	N3-C4-C5	5.39	131.30	128.60
32	2a	7	G	N3-C4-C5	5.39	131.30	128.60
32	2a	572	A	N1-C6-N6	-5.39	115.36	118.60
1	1A	478	A	N1-C2-N3	5.39	132.00	129.30
1	1A	689	A	OP1-P-O3'	5.39	117.06	105.20
1	1A	2036	C	N1-C2-O2	-5.39	115.66	118.90
1	1A	2315	G	N1-C6-O6	5.39	123.14	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	353	A	C5-C6-N6	-5.39	119.39	123.70
32	1a	979	C	C6-N1-C2	-5.39	118.14	120.30
32	1a	1380	U	O5'-P-OP2	-5.39	100.85	105.70
1	2A	888	C	C5-C6-N1	5.39	123.70	121.00
1	2A	1314	C	O5'-P-OP2	-5.39	100.85	105.70
1	2A	1606	G	N9-C4-C5	-5.39	103.24	105.40
1	2A	1688	U	C4-C5-C6	5.39	122.94	119.70
1	2A	2427	C	N3-C4-C5	5.39	124.06	121.90
2	2B	2	C	N1-C2-O2	5.39	122.14	118.90
1	1A	299	A	N7-C8-N9	-5.39	111.11	113.80
1	1A	841	A	C2-N3-C4	-5.39	107.91	110.60
1	1A	1837	C	O5'-P-OP1	-5.39	100.85	105.70
1	2A	1269	A	C2-N3-C4	-5.39	107.90	110.60
1	1A	802	A	C6-C5-N7	-5.39	128.53	132.30
1	1A	843	G	OP1-P-OP2	-5.39	111.52	119.60
1	1A	873	G	N1-C6-O6	5.39	123.13	119.90
1	1A	1379	A	N7-C8-N9	-5.39	111.11	113.80
1	1A	1634	A	O4'-C1'-N9	5.39	112.51	108.20
1	1A	1694	C	N3-C2-O2	5.39	125.67	121.90
32	1a	901	A	C4-C5-C6	5.39	119.69	117.00
1	2A	1334	G	N9-C4-C5	5.39	107.56	105.40
1	2A	2440	C	C5-C4-N4	5.39	123.97	120.20
18	2W	60	ASN	N-CA-CB	-5.39	100.90	110.60
1	1A	1232	G	N3-C2-N2	-5.39	116.13	119.90
1	1A	1430	C	N3-C4-N4	-5.39	114.23	118.00
1	1A	2179	C	C6-N1-C1'	-5.39	114.33	120.80
1	1A	2518	A	O5'-P-OP1	-5.39	100.85	105.70
32	1a	825	G	OP2-P-O3'	5.39	117.05	105.20
1	2A	2821	A	C5-C6-N1	-5.39	115.01	117.70
1	1A	366	C	C6-N1-C2	5.39	122.45	120.30
1	1A	2604	U	C4-C5-C6	5.39	122.93	119.70
1	1A	2714	G	OP1-P-OP2	5.39	127.68	119.60
1	2A	351	G	C4-N9-C1'	5.39	133.50	126.50
1	2A	1202	C	C5-C6-N1	-5.39	118.31	121.00
1	2A	1804	C	N3-C4-C5	5.39	124.06	121.90
1	2A	1963	U	OP1-P-O3'	5.39	117.05	105.20
1	2A	2008	C	C6-N1-C2	5.39	122.45	120.30
1	2A	2235	G	C5-C6-N1	-5.39	108.81	111.50
32	2a	560	U	O5'-P-OP1	-5.39	100.85	105.70
32	2a	659	U	N3-C4-O4	-5.39	115.63	119.40
32	2a	765	G	C6-C5-N7	-5.39	127.17	130.40
32	2a	1116	C	N1-C2-O2	5.39	122.13	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1435	G	N7-C8-N9	5.39	115.79	113.10
1	1A	300	A	C8-N9-C4	-5.38	103.65	105.80
1	1A	766	C	C5-C6-N1	-5.38	118.31	121.00
1	1A	805	G	C5-C6-N1	5.38	114.19	111.50
1	1A	1581	G	C4-N9-C1'	5.38	133.50	126.50
1	1A	1604	C	C5-C4-N4	-5.38	116.43	120.20
1	1A	2231	C	C5-C6-N1	-5.38	118.31	121.00
1	1A	2616	C	C2-N3-C4	-5.38	117.21	119.90
32	1a	879	C	C2-N1-C1'	-5.38	112.88	118.80
32	1a	1478	C	N3-C4-C5	5.38	124.05	121.90
1	2A	334	C	N3-C4-C5	-5.38	119.75	121.90
1	2A	775	G	N1-C6-O6	5.38	123.13	119.90
1	2A	1519	G	C8-N9-C4	-5.38	104.25	106.40
1	1A	1526	G	N1-C6-O6	5.38	123.13	119.90
2	1B	32	C	N3-C4-C5	5.38	124.05	121.90
32	1a	717	C	C5-C6-N1	5.38	123.69	121.00
1	2A	181	A	C2-N3-C4	-5.38	107.91	110.60
1	2A	2679	A	O5'-P-OP2	-5.38	100.86	105.70
1	1A	827	U	C6-N1-C1'	5.38	128.73	121.20
1	1A	1992	G	N7-C8-N9	-5.38	110.41	113.10
1	1A	2853	C	C5-C6-N1	-5.38	118.31	121.00
32	1a	1076	C	OP2-P-O3'	5.38	117.04	105.20
1	2A	512	G	C4-C5-N7	-5.38	108.65	110.80
1	2A	874	G	C8-N9-C1'	5.38	134.00	127.00
1	2A	1560	G	C2-N3-C4	-5.38	109.21	111.90
1	2A	2022	U	OP2-P-O3'	5.38	117.04	105.20
1	2A	2586	C	C5-C4-N4	-5.38	116.43	120.20
1	2A	2773	C	C4-C5-C6	5.38	120.09	117.40
2	2B	117	G	C5-C6-N1	-5.38	108.81	111.50
32	2a	1379	G	N1-C6-O6	-5.38	116.67	119.90
1	1A	79	G	C4-C5-N7	5.38	112.95	110.80
1	1A	1757	U	N3-C2-O2	5.38	125.97	122.20
1	2A	1840	G	C8-N9-C4	5.38	108.55	106.40
32	2a	399	G	C8-N9-C4	5.38	108.55	106.40
32	2a	579	G	C4-N9-C1'	5.38	133.49	126.50
32	2a	1149	C	C5-C6-N1	5.38	123.69	121.00
1	1A	189	G	N3-C4-N9	5.38	129.23	126.00
1	1A	622	G	C8-N9-C4	5.38	108.55	106.40
1	1A	1218	C	C6-N1-C2	5.38	122.45	120.30
32	1a	872	A	C4-C5-N7	5.38	113.39	110.70
1	2A	1187	G	N7-C8-N9	5.38	115.79	113.10
1	2A	1960	A	C8-N9-C4	5.38	107.95	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2031	A	C6-C5-N7	-5.38	128.53	132.30
1	2A	2134	A	N1-C6-N6	-5.38	115.37	118.60
1	2A	2712(A)	A	C5-N7-C8	-5.38	101.21	103.90
1	1A	1026	U	N1-C2-O2	5.38	126.56	122.80
1	1A	1958	C	OP1-P-OP2	-5.38	111.53	119.60
1	1A	2072	G	N1-C2-N3	-5.38	120.67	123.90
1	1A	2073	C	C6-N1-C2	5.38	122.45	120.30
1	1A	2102	U	C2-N3-C4	5.38	130.22	127.00
32	1a	587	G	N1-C6-O6	5.38	123.13	119.90
32	1a	783	C	N3-C4-N4	-5.38	114.24	118.00
1	2A	2494	G	N9-C4-C5	-5.38	103.25	105.40
1	2A	2645	G	C2-N3-C4	-5.38	109.21	111.90
32	2a	344	A	N1-C6-N6	5.38	121.83	118.60
1	1A	1195	G	N3-C4-N9	-5.38	122.78	126.00
1	1A	1343	G	OP2-P-O3'	5.38	117.03	105.20
32	1a	912	C	N3-C4-C5	-5.38	119.75	121.90
1	2A	1131	G	N1-C6-O6	5.38	123.12	119.90
32	2a	204	U	C2-N1-C1'	5.38	124.15	117.70
1	1A	134	C	OP1-P-OP2	-5.37	111.54	119.60
1	1A	376	C	C2-N1-C1'	-5.37	112.89	118.80
1	1A	2002	G	N9-C4-C5	-5.37	103.25	105.40
1	1A	2256	G	N1-C6-O6	-5.37	116.67	119.90
32	1a	668	G	N1-C6-O6	-5.37	116.68	119.90
32	1a	882	C	C5-C6-N1	5.37	123.69	121.00
32	1a	926	G	C4-C5-C6	5.37	122.03	118.80
1	2A	854	G	C5-C6-O6	5.37	131.82	128.60
1	2A	2414	G	N1-C6-O6	5.37	123.12	119.90
1	2A	2520	C	C2-N1-C1'	-5.37	112.89	118.80
1	2A	2842	G	O5'-P-OP1	5.37	117.15	110.70
32	2a	1103	C	C5-C6-N1	5.37	123.69	121.00
32	2a	1205	U	C5-C6-N1	5.37	125.39	122.70
1	1A	1343	G	N3-C4-C5	-5.37	125.92	128.60
1	1A	2432	A	C8-N9-C4	5.37	107.95	105.80
1	2A	1266	G	N7-C8-N9	-5.37	110.41	113.10
1	1A	271(B)	C	C5-C6-N1	-5.37	118.31	121.00
1	1A	727	A	C2-N3-C4	-5.37	107.92	110.60
1	1A	1656	C	C4-C5-C6	-5.37	114.72	117.40
1	1A	2331	G	N1-C6-O6	5.37	123.12	119.90
32	1a	817	C	N3-C2-O2	5.37	125.66	121.90
35	1d	135	LEU	CA-CB-CG	5.37	127.65	115.30
1	2A	582	G	N7-C8-N9	-5.37	110.42	113.10
1	2A	1838	C	C4-C5-C6	5.37	120.08	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1378	A	N7-C8-N9	-5.37	111.12	113.80
1	1A	1781	C	C6-N1-C2	5.37	122.45	120.30
1	1A	2293	C	N3-C2-O2	-5.37	118.14	121.90
32	1a	1151	A	C2-N3-C4	5.37	113.28	110.60
1	2A	733	G	N7-C8-N9	-5.37	110.42	113.10
1	2A	2014	A	O5'-P-OP2	5.37	117.14	110.70
1	2A	2143	C	N1-C2-O2	5.37	122.12	118.90
1	1A	1842	G	C4-C5-N7	5.37	112.95	110.80
12	1Q	67	ARG	NE-CZ-NH1	-5.37	117.62	120.30
1	2A	2247	A	C4-C5-C6	5.37	119.68	117.00
1	1A	40	C	N3-C2-O2	5.37	125.66	121.90
1	1A	146	G	C4-C5-N7	5.37	112.95	110.80
1	1A	398	G	C2-N3-C4	-5.37	109.22	111.90
1	1A	443	A	N1-C6-N6	-5.37	115.38	118.60
1	1A	814	C	OP1-P-OP2	-5.37	111.55	119.60
1	1A	1817	G	C2-N3-C4	5.37	114.58	111.90
1	1A	2817	G	C5-N7-C8	-5.37	101.62	104.30
1	2A	693	C	N3-C2-O2	5.37	125.66	121.90
1	2A	1207	C	O5'-P-OP1	-5.37	100.87	105.70
32	2a	1053	G	C4-N9-C1'	-5.37	119.53	126.50
1	1A	562	U	O5'-P-OP1	-5.36	100.87	105.70
1	1A	762	U	N3-C4-O4	5.36	123.15	119.40
1	1A	997	G	C8-N9-C4	5.36	108.55	106.40
1	1A	1668	A	N1-C2-N3	5.36	131.98	129.30
1	1A	1786	A	C6-N1-C2	-5.36	115.38	118.60
1	1A	1952	A	C5-C6-N1	-5.36	115.02	117.70
32	1a	1472	U	N3-C2-O2	5.36	125.95	122.20
1	2A	465	G	OP1-P-OP2	-5.36	111.56	119.60
1	2A	504	U	C6-N1-C1'	-5.36	113.69	121.20
1	2A	1692	U	O5'-P-OP2	-5.36	100.87	105.70
1	2A	1888	G	C6-C5-N7	-5.36	127.18	130.40
2	2B	57	A	O5'-P-OP2	-5.36	100.87	105.70
32	2a	518	C	C2-N1-C1'	5.36	124.70	118.80
32	2a	1486	G	C8-N9-C4	5.36	108.55	106.40
1	1A	530	G	C2-N3-C4	5.36	114.58	111.90
1	1A	1595	G	O5'-P-OP1	-5.36	100.87	105.70
1	1A	2040	C	N3-C2-O2	5.36	125.65	121.90
32	1a	1158	C	N3-C4-C5	-5.36	119.75	121.90
1	2A	1840	G	O5'-P-OP1	-5.36	100.87	105.70
1	2A	2107	C	C5-C6-N1	5.36	123.68	121.00
32	2a	626	U	C5-C6-N1	-5.36	120.02	122.70
1	1A	1066	U	C6-N1-C2	-5.36	117.78	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1181	G	C6-N1-C2	5.36	128.32	125.10
1	2A	729	G	OP2-P-O3'	5.36	116.99	105.20
1	2A	766	C	C4-C5-C6	5.36	120.08	117.40
1	2A	1524	G	N3-C2-N2	-5.36	116.15	119.90
1	2A	1777	U	C5-C6-N1	-5.36	120.02	122.70
1	2A	2373	G	C8-N9-C4	5.36	108.54	106.40
1	2A	2744	G	C4-C5-N7	5.36	112.94	110.80
32	2a	576	G	C6-C5-N7	-5.36	127.18	130.40
1	2A	2394	C	N3-C2-O2	-5.36	118.15	121.90
1	2A	2596	U	O5'-P-OP2	-5.36	100.88	105.70
1	1A	428	A	C6-C5-N7	-5.36	128.55	132.30
1	1A	599	G	N9-C4-C5	-5.36	103.26	105.40
1	1A	783	A	C5-N7-C8	-5.36	101.22	103.90
1	1A	1643	G	C4-C5-N7	-5.36	108.66	110.80
1	1A	1864	U	C4-C5-C6	5.36	122.92	119.70
1	1A	2646	C	N3-C4-N4	5.36	121.75	118.00
29	17	47	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	2A	584	C	N3-C4-N4	5.36	121.75	118.00
1	2A	682	G	C4-N9-C1'	5.36	133.46	126.50
1	2A	1992	G	C8-N9-C4	5.36	108.54	106.40
1	2A	2187	G	C6-C5-N7	-5.36	127.19	130.40
1	2A	2378	A	N1-C2-N3	5.36	131.98	129.30
1	2A	2587	A	N1-C6-N6	5.36	121.81	118.60
32	2a	525	C	N3-C4-N4	5.36	121.75	118.00
32	2a	1026	G	C8-N9-C4	-5.36	104.26	106.40
1	1A	103	A	C2-N3-C4	-5.36	107.92	110.60
1	1A	859	G	N7-C8-N9	-5.36	110.42	113.10
1	1A	1810	A	C6-C5-N7	-5.36	128.55	132.30
1	1A	2197	U	C6-N1-C2	5.36	124.21	121.00
1	1A	2614	A	N1-C6-N6	-5.36	115.39	118.60
17	1V	13	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	2A	268	C	C6-N1-C2	-5.36	118.16	120.30
1	2A	1598	C	C5-C6-N1	-5.36	118.32	121.00
1	2A	1688	U	C6-N1-C2	-5.36	117.79	121.00
1	2A	1827	C	N3-C2-O2	-5.36	118.15	121.90
1	2A	2365	G	O5'-P-OP2	-5.36	100.88	105.70
1	1A	77	C	N3-C4-C5	5.35	124.04	121.90
1	1A	532	A	N1-C6-N6	-5.35	115.39	118.60
1	1A	1002	G	N3-C2-N2	-5.35	116.15	119.90
1	1A	1477	A	OP1-P-OP2	5.35	127.63	119.60
1	1A	1900	A	N9-C4-C5	5.35	107.94	105.80
1	1A	2554	U	N1-C2-O2	-5.35	119.05	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1B	102	A	C8-N9-C1'	-5.35	118.06	127.70
1	2A	614(A)	U	O5'-P-OP2	-5.35	100.88	105.70
1	1A	516	C	C5-C4-N4	-5.35	116.45	120.20
1	1A	665	C	O5'-P-OP1	5.35	117.12	110.70
1	1A	926	A	C5-C6-N6	-5.35	119.42	123.70
1	1A	1328	G	N3-C4-C5	-5.35	125.92	128.60
1	1A	1553	A	N9-C4-C5	-5.35	103.66	105.80
1	1A	2031	A	N9-C4-C5	5.35	107.94	105.80
1	2A	2268	A	O5'-P-OP1	-5.35	100.88	105.70
1	2A	2321	G	C8-N9-C1'	-5.35	120.04	127.00
1	2A	2576	G	N3-C4-C5	-5.35	125.92	128.60
32	2a	517	G	C5-C6-O6	5.35	131.81	128.60
32	2a	689	C	N3-C4-C5	-5.35	119.76	121.90
32	2a	1406	U	O5'-P-OP2	-5.35	100.88	105.70
1	1A	59	U	C6-N1-C2	-5.35	117.79	121.00
13	1R	12	ARG	NE-CZ-NH1	-5.35	117.62	120.30
32	1a	1075	C	O5'-P-OP1	-5.35	100.88	105.70
1	2A	527	C	N1-C2-O2	-5.35	115.69	118.90
1	2A	655	A	C4-C5-C6	5.35	119.67	117.00
1	1A	299	A	C8-N9-C4	5.35	107.94	105.80
1	1A	940	G	N3-C4-C5	-5.35	125.92	128.60
1	1A	983	A	OP1-P-O3'	-5.35	93.43	105.20
1	1A	1170	G	N1-C6-O6	5.35	123.11	119.90
1	1A	1841	U	N3-C4-O4	-5.35	115.66	119.40
1	1A	2426	A	N1-C6-N6	-5.35	115.39	118.60
1	1A	2624	G	N3-C4-C5	5.35	131.28	128.60
1	1A	2719	G	C2-N3-C4	5.35	114.58	111.90
1	1A	2741	A	C2-N3-C4	-5.35	107.92	110.60
1	1A	2810	A	C5-N7-C8	-5.35	101.22	103.90
32	1a	904	C	C5-C6-N1	-5.35	118.33	121.00
1	2A	993	G	C4-N9-C1'	-5.35	119.54	126.50
1	2A	1404	C	C5-C4-N4	5.35	123.94	120.20
1	2A	2142	C	C6-N1-C2	-5.35	118.16	120.30
1	1A	139(A)	G	OP1-P-OP2	5.35	127.62	119.60
1	1A	213	A	N1-C6-N6	5.35	121.81	118.60
1	1A	1681	G	C5-C6-N1	5.35	114.17	111.50
1	1A	2019	A	C5-C6-N6	-5.35	119.42	123.70
1	1A	2068	U	N1-C2-O2	-5.35	119.06	122.80
32	1a	633	G	N3-C4-N9	-5.35	122.79	126.00
1	2A	461	C	C6-N1-C2	-5.35	118.16	120.30
1	2A	2224	G	C5-C6-N1	-5.35	108.83	111.50
1	1A	880	G	N3-C4-C5	-5.35	125.93	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1843	C	C5-C4-N4	-5.35	116.46	120.20
1	1A	2664	G	C4-C5-N7	-5.35	108.66	110.80
32	1a	353	A	C5-N7-C8	-5.35	101.23	103.90
32	1a	1354	C	N3-C2-O2	-5.35	118.16	121.90
1	2A	2241	A	N9-C4-C5	5.35	107.94	105.80
32	2a	520	A	N9-C4-C5	5.35	107.94	105.80
1	1A	242	G	C4-C5-N7	5.34	112.94	110.80
1	1A	1097	U	C6-N1-C2	-5.34	117.79	121.00
1	1A	2445	G	C4-C5-N7	-5.34	108.66	110.80
1	1A	2639	A	C5-C6-N6	-5.34	119.42	123.70
32	1a	297	G	C8-N9-C4	5.34	108.54	106.40
32	1a	1244	C	C6-N1-C2	-5.34	118.16	120.30
1	2A	59	U	C6-N1-C2	-5.34	117.79	121.00
1	2A	648	G	C5-C6-N1	-5.34	108.83	111.50
1	2A	1307	A	N7-C8-N9	-5.34	111.13	113.80
1	2A	1333	C	N1-C2-O2	5.34	122.11	118.90
1	2A	2302	G	C8-N9-C4	-5.34	104.26	106.40
32	1a	784	C	N3-C2-O2	-5.34	118.16	121.90
32	1a	1285	A	P-O3'-C3'	5.34	126.11	119.70
32	2a	354	G	N7-C8-N9	5.34	115.77	113.10
32	2a	1061	G	N7-C8-N9	5.34	115.77	113.10
1	1A	270	A	N7-C8-N9	-5.34	111.13	113.80
1	1A	746	A	O4'-C1'-N9	5.34	112.47	108.20
1	1A	806	C	N1-C2-N3	-5.34	115.46	119.20
1	1A	1434	A	N9-C4-C5	5.34	107.94	105.80
1	1A	1605	C	OP2-P-O3'	5.34	116.95	105.20
1	1A	2747	G	C5-C6-O6	-5.34	125.39	128.60
2	1B	75	G	C8-N9-C1'	-5.34	120.06	127.00
1	2A	330	A	C5-C6-N6	-5.34	119.43	123.70
1	2A	1606	G	C8-N9-C1'	-5.34	120.06	127.00
1	2A	2699	C	C6-N1-C2	5.34	122.44	120.30
32	2a	282	A	C5-N7-C8	-5.34	101.23	103.90
1	1A	244	A	C5-C6-N6	-5.34	119.43	123.70
1	1A	619	G	C4-C5-N7	5.34	112.94	110.80
1	1A	968	G	N9-C4-C5	5.34	107.54	105.40
1	1A	1631	C	N3-C4-C5	-5.34	119.76	121.90
1	1A	2310	A	C8-N9-C4	-5.34	103.66	105.80
1	1A	2376	A	N1-C6-N6	-5.34	115.40	118.60
1	1A	2418	A	N9-C4-C5	-5.34	103.66	105.80
2	1B	71	C	C4-C5-C6	5.34	120.07	117.40
32	1a	595	G	C8-N9-C1'	-5.34	120.06	127.00
1	2A	871	U	O5'-P-OP1	-5.34	100.89	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1991	U	N3-C4-O4	-5.34	115.66	119.40
1	2A	2061	G	C5-N7-C8	-5.34	101.63	104.30
1	2A	2108	C	C6-N1-C2	-5.34	118.16	120.30
1	1A	805	G	N7-C8-N9	5.34	115.77	113.10
1	1A	2269	A	C2-N3-C4	-5.34	107.93	110.60
1	1A	2356	C	C6-N1-C1'	5.34	127.20	120.80
1	1A	2678	C	C4-C5-C6	5.34	120.07	117.40
32	2a	622	A	N1-C6-N6	-5.34	115.40	118.60
1	1A	428	A	N1-C2-N3	5.34	131.97	129.30
1	1A	748	G	OP1-P-O3'	5.34	116.94	105.20
1	1A	802	A	C4-C5-C6	5.34	119.67	117.00
1	1A	940	G	C2-N3-C4	5.34	114.57	111.90
1	1A	1155	A	O5'-P-OP2	-5.34	100.90	105.70
12	1Q	103	MET	CG-SD-CE	-5.34	91.66	100.20
32	1a	562	C	O5'-P-OP2	-5.34	100.90	105.70
32	1a	875	C	OP1-P-O3'	5.34	116.94	105.20
1	2A	601	C	OP2-P-O3'	5.34	116.94	105.20
1	2A	694	U	C5-C4-O4	5.34	129.10	125.90
1	2A	866	A	C8-N9-C4	5.34	107.94	105.80
1	2A	1775	U	OP1-P-O3'	5.34	116.94	105.20
1	2A	2458	G	N3-C4-C5	-5.34	125.93	128.60
32	2a	1483	A	C8-N9-C4	5.34	107.93	105.80
1	1A	997	G	C5-N7-C8	5.33	106.97	104.30
1	1A	1225	G	OP2-P-O3'	5.33	116.94	105.20
1	1A	2090	G	OP1-P-OP2	5.33	127.60	119.60
1	1A	2485	G	N9-C4-C5	-5.33	103.27	105.40
4	1E	154	LYS	CD-CE-NZ	-5.33	99.43	111.70
1	2A	1076	C	C5-C6-N1	5.33	123.67	121.00
1	2A	1890	A	N7-C8-N9	-5.33	111.13	113.80
1	1A	57	C	N1-C2-O2	-5.33	115.70	118.90
1	1A	1093	G	O4'-C1'-N9	5.33	112.47	108.20
1	1A	1215	G	C5-C6-O6	-5.33	125.40	128.60
1	1A	1390	U	N3-C2-O2	5.33	125.93	122.20
1	1A	1633	G	C8-N9-C4	-5.33	104.27	106.40
1	1A	1648	C	C5-C6-N1	-5.33	118.33	121.00
1	1A	1927	A	N7-C8-N9	5.33	116.47	113.80
1	1A	2454	G	C5-C6-O6	5.33	131.80	128.60
1	1A	2725	A	O5'-P-OP2	-5.33	100.90	105.70
32	1a	758	G	C5-N7-C8	-5.33	101.63	104.30
32	1a	819	A	O5'-P-OP1	-5.33	100.90	105.70
1	2A	1633	G	C2-N3-C4	5.33	114.57	111.90
1	2A	1791	A	N7-C8-N9	5.33	116.47	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1826	G	N1-C2-N3	5.33	127.10	123.90
1	2A	1941	C	O5'-P-OP1	-5.33	100.90	105.70
1	2A	2042	A	N3-C4-C5	5.33	130.53	126.80
32	2a	298	A	N1-C6-N6	-5.33	115.40	118.60
1	1A	570	G	C4-C5-C6	-5.33	115.60	118.80
1	1A	2394	C	C5-C4-N4	-5.33	116.47	120.20
32	1a	458	C	C6-N1-C2	-5.33	118.17	120.30
32	1a	1516	G	C8-N9-C1'	5.33	133.93	127.00
1	2A	242	G	C4-N9-C1'	-5.33	119.57	126.50
1	2A	456	C	C6-N1-C1'	-5.33	114.40	120.80
1	2A	1471	A	C6-C5-N7	-5.33	128.57	132.30
1	2A	2497	A	C5-N7-C8	5.33	106.57	103.90
1	2A	2789	C	O4'-C1'-N1	5.33	112.47	108.20
32	2a	334	C	N3-C4-C5	5.33	124.03	121.90
32	2a	1432	G	C5-N7-C8	5.33	106.97	104.30
1	1A	1105	U	C5-C4-O4	-5.33	122.70	125.90
1	1A	1583	A	O5'-P-OP2	-5.33	100.90	105.70
1	2A	734	A	N1-C2-N3	5.33	131.97	129.30
1	1A	125	G	C5-C6-O6	-5.33	125.40	128.60
1	1A	2240	C	C5-C6-N1	-5.33	118.34	121.00
32	1a	423	G	N3-C4-N9	5.33	129.20	126.00
32	1a	536	C	C6-N1-C2	-5.33	118.17	120.30
1	2A	29	U	N1-C2-O2	5.33	126.53	122.80
1	2A	493	G	C4-C5-N7	5.33	112.93	110.80
1	2A	527	C	C4-C5-C6	5.33	120.06	117.40
1	2A	783	A	C8-N9-C4	-5.33	103.67	105.80
1	2A	1078	U	C5-C4-O4	-5.33	122.70	125.90
1	2A	1552	G	N3-C4-N9	-5.33	122.80	126.00
1	2A	2063	C	OP1-P-O3'	-5.33	93.48	105.20
1	2A	2187	G	C4-N9-C1'	5.33	133.43	126.50
2	2B	74	U	C4-C5-C6	5.33	122.90	119.70
32	2a	1045	C	N1-C2-O2	5.33	122.10	118.90
1	1A	794	G	OP2-P-O3'	5.33	116.92	105.20
1	1A	1062	G	C5-C6-O6	-5.33	125.40	128.60
1	1A	2278	A	C6-C5-N7	-5.33	128.57	132.30
1	1A	2895	U	C6-N1-C2	-5.33	117.80	121.00
32	1a	552	U	C2-N1-C1'	-5.33	111.31	117.70
1	2A	774	A	N1-C6-N6	5.33	121.80	118.60
1	1A	186	G	N7-C8-N9	-5.33	110.44	113.10
1	1A	1036	G	N7-C8-N9	-5.33	110.44	113.10
1	1A	1627	G	OP1-P-OP2	5.33	127.59	119.60
1	1A	2242	G	C5-C6-N1	-5.33	108.84	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2615	U	N1-C2-O2	5.33	126.53	122.80
32	1a	472	A	C8-N9-C4	-5.33	103.67	105.80
2	2B	51	G	N3-C4-C5	-5.33	125.94	128.60
1	1A	123	G	O5'-P-OP1	5.32	117.09	110.70
1	1A	401	A	OP2-P-O3'	5.32	116.91	105.20
1	1A	533	G	N1-C6-O6	5.32	123.09	119.90
1	1A	932	G	C4-C5-N7	-5.32	108.67	110.80
1	1A	965	C	C5-C4-N4	-5.32	116.47	120.20
1	1A	1364	G	N1-C6-O6	-5.32	116.71	119.90
1	1A	1804	C	C4-C5-C6	5.32	120.06	117.40
1	1A	2718	G	C6-C5-N7	-5.32	127.21	130.40
1	1A	2813	A	N1-C2-N3	5.32	131.96	129.30
1	2A	955	C	N1-C2-O2	-5.32	115.71	118.90
1	2A	1772	G	O4'-C1'-N9	5.32	112.46	108.20
1	2A	2498	C	N1-C2-O2	-5.32	115.71	118.90
1	2A	2709	G	C4-C5-C6	-5.32	115.61	118.80
32	2a	100	C	C6-N1-C2	-5.32	118.17	120.30
32	2a	991	U	P-O3'-C3'	5.32	126.09	119.70
1	1A	655	A	N1-C2-N3	5.32	131.96	129.30
1	1A	1990	C	N1-C2-N3	5.32	122.93	119.20
1	1A	2440	C	C6-N1-C2	5.32	122.43	120.30
1	1A	2446	G	P-O3'-C3'	5.32	126.09	119.70
32	1a	481	G	C6-C5-N7	-5.32	127.21	130.40
32	1a	809	G	N3-C4-C5	5.32	131.26	128.60
1	2A	219	G	N3-C4-C5	-5.32	125.94	128.60
1	2A	1425	G	C2-N3-C4	-5.32	109.24	111.90
1	2A	2765	A	C4-C5-N7	5.32	113.36	110.70
13	2R	103	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	1A	271	A	N7-C8-N9	-5.32	111.14	113.80
1	1A	666	G	C8-N9-C4	5.32	108.53	106.40
1	1A	2271	G	N3-C4-N9	5.32	129.19	126.00
17	1V	83	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	2A	470	A	C4-C5-N7	5.32	113.36	110.70
1	2A	2042	A	C2-N3-C4	-5.32	107.94	110.60
32	2a	412	A	N9-C4-C5	-5.32	103.67	105.80
32	2a	1460	A	C8-N9-C4	5.32	107.93	105.80
1	1A	28	A	C5-C6-N6	-5.32	119.44	123.70
1	1A	1264	G	P-O3'-C3'	5.32	126.08	119.70
1	1A	1853	A	N9-C4-C5	5.32	107.93	105.80
1	1A	98	G	OP1-P-OP2	5.32	127.58	119.60
1	1A	312	G	C8-N9-C4	-5.32	104.27	106.40
1	1A	679	C	OP2-P-O3'	5.32	116.90	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1216	G	C5-N7-C8	5.32	106.96	104.30
1	1A	1625	C	OP1-P-O3'	5.32	116.90	105.20
1	1A	1777	U	C6-N1-C1'	-5.32	113.76	121.20
1	1A	2179	C	C2-N3-C4	5.32	122.56	119.90
1	1A	2411	A	C5-N7-C8	-5.32	101.24	103.90
1	1A	2462	U	C6-N1-C2	5.32	124.19	121.00
1	2A	2202	C	O5'-P-OP1	5.32	117.08	110.70
1	2A	2421	G	C4-N9-C1'	5.32	133.41	126.50
32	2a	1074	G	N1-C6-O6	5.32	123.09	119.90
1	1A	831	G	OP1-P-O3'	5.32	116.90	105.20
1	1A	1257	C	C6-N1-C2	-5.32	118.17	120.30
1	1A	1520	G	C4-C5-N7	-5.32	108.67	110.80
25	13	8	LEU	CB-CG-CD1	-5.32	101.97	111.00
32	1a	995	C	C6-N1-C2	-5.32	118.17	120.30
2	2B	47	C	O4'-C1'-N1	5.32	112.45	108.20
32	2a	354	G	C8-N9-C4	-5.32	104.27	106.40
1	2A	233	A	O5'-P-OP2	-5.31	100.92	105.70
1	1A	513	A	N9-C4-C5	-5.31	103.67	105.80
1	1A	792	G	N3-C4-N9	5.31	129.19	126.00
1	1A	1603	A	C5-N7-C8	-5.31	101.24	103.90
1	1A	1695	G	C2-N3-C4	-5.31	109.24	111.90
1	1A	2040	C	C2-N3-C4	5.31	122.56	119.90
1	1A	2062	A	N3-C4-C5	5.31	130.52	126.80
1	1A	2838	G	C4-C5-N7	5.31	112.92	110.80
1	1A	2847	U	O4'-C1'-N1	5.31	112.45	108.20
1	2A	23	G	C8-N9-C4	5.31	108.53	106.40
1	2A	982	C	C2-N3-C4	5.31	122.56	119.90
1	2A	1178	C	C5-C6-N1	5.31	123.66	121.00
1	2A	1191	G	C8-N9-C4	5.31	108.53	106.40
1	2A	1940	U	C5-C4-O4	-5.31	122.71	125.90
32	2a	391	G	C5-N7-C8	-5.31	101.64	104.30
1	1A	416	C	N3-C4-N4	-5.31	114.28	118.00
1	1A	993	G	OP1-P-OP2	-5.31	111.63	119.60
1	1A	1208	C	C5-C6-N1	-5.31	118.34	121.00
1	1A	1252	G	OP1-P-O3'	5.31	116.88	105.20
1	1A	2280	G	OP1-P-O3'	5.31	116.88	105.20
1	1A	2628	C	C4-C5-C6	5.31	120.06	117.40
1	1A	2665	A	C5-C6-N6	5.31	127.95	123.70
1	1A	2712(A)	A	N1-C6-N6	5.31	121.79	118.60
32	1a	23	C	O5'-P-OP2	-5.31	100.92	105.70
1	2A	1776	G	N7-C8-N9	5.31	115.75	113.10
1	2A	2468	G	O4'-C1'-N9	5.31	112.45	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	631	G	N3-C4-C5	5.31	131.25	128.60
32	2a	721	G	C4-N9-C1'	5.31	133.40	126.50
1	1A	199	A	C5-C6-N1	5.31	120.35	117.70
1	1A	351	G	N3-C2-N2	-5.31	116.19	119.90
1	1A	1338	G	N3-C4-N9	5.31	129.19	126.00
1	1A	2516	G	C8-N9-C4	-5.31	104.28	106.40
32	1a	672	U	O5'-P-OP1	-5.31	100.92	105.70
32	1a	766	A	N9-C4-C5	-5.31	103.68	105.80
2	2B	56	G	OP2-P-O3'	5.31	116.88	105.20
32	2a	59	A	C4-C5-N7	5.31	113.35	110.70
1	1A	1886	C	C6-N1-C2	5.31	122.42	120.30
1	1A	2334	G	N3-C4-N9	5.31	129.18	126.00
1	2A	2442	C	N3-C4-N4	5.31	121.71	118.00
1	2A	2622	C	C2-N1-C1'	-5.31	112.96	118.80
1	1A	51	G	C4-C5-N7	-5.30	108.68	110.80
1	1A	1004	C	C5-C4-N4	5.30	123.91	120.20
1	1A	2658	C	O5'-P-OP1	-5.30	100.93	105.70
32	1a	277	C	C5-C6-N1	-5.30	118.35	121.00
32	1a	772	U	N3-C2-O2	5.30	125.91	122.20
1	2A	1838	C	N1-C2-N3	5.30	122.91	119.20
32	2a	1418	A	C6-C5-N7	-5.30	128.59	132.30
32	2a	1468	A	N1-C6-N6	5.30	121.78	118.60
1	1A	2789	C	C5-C4-N4	5.30	123.91	120.20
1	2A	2206	G	C8-N9-C4	5.30	108.52	106.40
32	2a	704	A	C8-N9-C4	-5.30	103.68	105.80
1	1A	1086	A	C8-N9-C4	-5.30	103.68	105.80
1	1A	1163	G	N1-C6-O6	5.30	123.08	119.90
1	1A	1566	A	C4-C5-C6	-5.30	114.35	117.00
1	1A	1948	G	O5'-P-OP1	-5.30	100.93	105.70
1	1A	2873	A	N1-C6-N6	5.30	121.78	118.60
32	1a	576	G	C5-C6-N1	-5.30	108.85	111.50
32	1a	1504	G	OP2-P-O3'	5.30	116.86	105.20
1	2A	1603	A	OP1-P-O3'	5.30	116.86	105.20
1	2A	1978	A	C2-N3-C4	-5.30	107.95	110.60
1	2A	2084	C	N3-C2-O2	5.30	125.61	121.90
32	2a	511	C	C6-N1-C1'	5.30	127.16	120.80
32	2a	572	A	C4-N9-C1'	-5.30	116.76	126.30
1	1A	207	A	N7-C8-N9	5.30	116.45	113.80
1	1A	655	A	C6-C5-N7	-5.30	128.59	132.30
1	1A	1334	G	O5'-P-OP2	-5.30	100.93	105.70
1	1A	1847	A	C4-C5-C6	5.30	119.65	117.00
1	1A	2256	G	C5-C6-O6	5.30	131.78	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2707	G	N9-C4-C5	-5.30	103.28	105.40
32	1a	734	G	N3-C4-N9	5.30	129.18	126.00
1	2A	1959	G	C4-C5-N7	-5.30	108.68	110.80
1	1A	1792	G	N3-C4-C5	5.30	131.25	128.60
1	1A	2107	C	C2-N3-C4	5.30	122.55	119.90
1	1A	2645	G	C5-N7-C8	-5.30	101.65	104.30
1	1A	2856	C	O5'-P-OP1	-5.30	100.93	105.70
3	1D	229	VAL	CB-CA-C	-5.30	101.33	111.40
1	2A	1626	G	N3-C2-N2	-5.30	116.19	119.90
1	2A	1940	U	C2-N1-C1'	5.30	124.06	117.70
1	2A	2447	G	C6-N1-C2	-5.30	121.92	125.10
1	1A	297	C	N3-C4-C5	-5.30	119.78	121.90
1	1A	725	G	N3-C4-C5	-5.30	125.95	128.60
1	1A	1429	G	N1-C6-O6	-5.30	116.72	119.90
1	1A	1750	G	C5-C6-O6	-5.30	125.42	128.60
1	1A	2240	C	C5-C4-N4	-5.30	116.49	120.20
1	1A	2645	G	N3-C2-N2	5.30	123.61	119.90
32	1a	251	G	C2-N3-C4	5.30	114.55	111.90
32	1a	413	G	C4-C5-N7	-5.30	108.68	110.80
32	1a	804	U	C5-C4-O4	5.30	129.08	125.90
1	2A	15	G	N1-C6-O6	5.30	123.08	119.90
1	2A	1783	A	OP1-P-O3'	5.30	116.85	105.20
1	2A	2139	C	C6-N1-C2	-5.30	118.18	120.30
1	2A	2611	U	N3-C4-O4	5.30	123.11	119.40
1	2A	2701	C	N1-C2-O2	5.30	122.08	118.90
32	2a	142	G	N3-C4-C5	-5.30	125.95	128.60
32	2a	768	A	C8-N9-C4	5.30	107.92	105.80
32	2a	1201	A	P-O3'-C3'	5.30	126.06	119.70
1	1A	2061	G	N3-C2-N2	5.29	123.61	119.90
1	2A	127	A	C5-C6-N6	-5.29	119.46	123.70
1	2A	2238	G	N7-C8-N9	5.29	115.75	113.10
32	2a	980	C	C2-N1-C1'	5.29	124.62	118.80
1	1A	1612	C	N3-C4-C5	5.29	124.02	121.90
1	1A	1651	G	N3-C4-N9	5.29	129.18	126.00
1	1A	2687	U	N3-C4-O4	5.29	123.11	119.40
32	1a	542	G	OP1-P-O3'	5.29	116.84	105.20
1	2A	1461	G	C5-C6-O6	5.29	131.78	128.60
15	2T	103	ARG	NE-CZ-NH1	-5.29	117.65	120.30
32	2a	78	G	N7-C8-N9	5.29	115.75	113.10
1	1A	154(A)	C	C4-C5-C6	-5.29	114.75	117.40
1	1A	1856	G	C2-N3-C4	-5.29	109.25	111.90
32	1a	1335	C	C6-N1-C2	5.29	122.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	330	A	N1-C2-N3	5.29	131.94	129.30
1	2A	2248	C	N3-C2-O2	-5.29	118.20	121.90
1	2A	2301	C	C6-N1-C2	-5.29	118.18	120.30
1	2A	2683	C	N3-C4-N4	5.29	121.70	118.00
2	2B	50	G	O5'-P-OP2	-5.29	100.94	105.70
34	2c	101	LEU	CA-CB-CG	5.29	127.47	115.30
1	1A	945	A	O4'-C1'-N9	-5.29	103.97	108.20
1	1A	1361	G	OP2-P-O3'	5.29	116.84	105.20
1	1A	2009	G	C4-N9-C1'	-5.29	119.62	126.50
32	1a	786	G	N1-C6-O6	5.29	123.07	119.90
1	1A	271(V)	G	C2-N3-C4	-5.29	109.26	111.90
1	1A	2444	G	OP1-P-OP2	5.29	127.53	119.60
1	1A	2669	G	N3-C2-N2	-5.29	116.20	119.90
2	1B	89	G	N9-C4-C5	-5.29	103.28	105.40
2	1B	102	A	C5-C6-N6	-5.29	119.47	123.70
32	1a	880	C	N3-C4-C5	5.29	124.02	121.90
1	1A	70	G	N3-C4-C5	-5.29	125.96	128.60
1	1A	1332	G	N3-C4-N9	5.29	129.17	126.00
1	1A	2539	C	N3-C4-N4	-5.29	114.30	118.00
32	2a	1030(C)	G	C8-N9-C4	-5.29	104.28	106.40
1	1A	777	A	C4-C5-N7	-5.29	108.06	110.70
1	1A	793	A	O5'-P-OP1	5.29	117.04	110.70
1	1A	832	G	C8-N9-C4	-5.29	104.29	106.40
1	1A	2098	U	O5'-P-OP1	-5.29	100.94	105.70
1	1A	2218	U	C2-N1-C1'	5.29	124.04	117.70
32	1a	622	A	C8-N9-C4	-5.29	103.69	105.80
1	1A	110	G	N7-C8-N9	-5.28	110.46	113.10
1	1A	545	G	N1-C2-N3	-5.28	120.73	123.90
1	1A	593	G	N1-C6-O6	5.28	123.07	119.90
1	1A	665	C	C6-N1-C2	5.28	122.41	120.30
1	1A	1149	G	O5'-P-OP1	5.28	117.04	110.70
1	1A	1893	C	C6-N1-C2	5.28	122.41	120.30
32	1a	895	G	C5-C6-N1	-5.28	108.86	111.50
32	1a	968	A	OP1-P-OP2	5.28	127.53	119.60
32	1a	1070	U	C6-N1-C2	-5.28	117.83	121.00
1	2A	874	G	C4-N9-C1'	-5.28	119.63	126.50
1	2A	1146	C	C6-N1-C2	-5.28	118.19	120.30
20	2Y	99	CYS	CA-CB-SG	5.28	123.51	114.00
32	2a	226	G	C4-C5-N7	-5.28	108.69	110.80
1	1A	1622	G	N1-C2-N2	5.28	120.95	116.20
1	1A	2190	G	N1-C6-O6	5.28	123.07	119.90
1	2A	1655	A	OP2-P-O3'	5.28	116.82	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	307	G	C4-N9-C1'	5.28	133.37	126.50
1	1A	391	G	C8-N9-C4	5.28	108.51	106.40
1	1A	590	A	C5-C6-N1	5.28	120.34	117.70
1	1A	1064	C	N3-C2-O2	-5.28	118.20	121.90
1	1A	1198	U	O5'-P-OP1	5.28	117.04	110.70
1	1A	1414	G	N3-C2-N2	-5.28	116.20	119.90
1	1A	1544	A	C5-N7-C8	5.28	106.54	103.90
1	1A	2359	C	N1-C2-O2	-5.28	115.73	118.90
1	2A	214	G	N7-C8-N9	-5.28	110.46	113.10
1	2A	2585	U	C6-N1-C1'	-5.28	113.81	121.20
32	2a	647	C	C5-C6-N1	5.28	123.64	121.00
1	1A	1655	A	OP2-P-O3'	5.28	116.81	105.20
1	2A	2307	G	N3-C4-N9	5.28	129.17	126.00
1	1A	224	G	N7-C8-N9	-5.28	110.46	113.10
1	1A	726	G	O5'-P-OP1	-5.28	100.95	105.70
1	1A	1965	C	N3-C4-C5	5.28	124.01	121.90
32	1a	1019	C	C6-N1-C2	-5.28	118.19	120.30
1	2A	741	G	N9-C4-C5	5.28	107.51	105.40
1	2A	1298	C	C6-N1-C2	-5.28	118.19	120.30
1	2A	1932	A	C6-C5-N7	-5.28	128.60	132.30
1	2A	2419	U	OP1-P-O3'	5.28	116.81	105.20
1	2A	2639	A	N1-C6-N6	5.28	121.77	118.60
32	2a	1163	C	C5-C6-N1	5.28	123.64	121.00
32	2a	1216	G	O5'-P-OP2	-5.28	100.95	105.70
1	1A	132	G	C4-C5-N7	-5.28	108.69	110.80
1	1A	1286	A	N9-C4-C5	5.28	107.91	105.80
1	1A	1708	C	OP1-P-OP2	5.28	127.51	119.60
1	1A	1830	C	OP2-P-O3'	5.28	116.80	105.20
32	1a	1281	U	C6-N1-C2	-5.28	117.83	121.00
1	1A	697	C	OP1-P-OP2	5.27	127.51	119.60
1	1A	1268	A	OP1-P-OP2	-5.27	111.69	119.60
1	1A	2112	G	C8-N9-C4	-5.27	104.29	106.40
1	1A	2534	A	N3-C4-C5	-5.27	123.11	126.80
1	1A	2872	G	C4-C5-C6	5.27	121.96	118.80
32	1a	1504	G	N7-C8-N9	-5.27	110.46	113.10
1	2A	915	C	N3-C2-O2	-5.27	118.21	121.90
1	1A	53	A	N1-C2-N3	5.27	131.94	129.30
1	1A	1047	G	P-O3'-C3'	5.27	126.03	119.70
1	1A	1387	C	C6-N1-C2	-5.27	118.19	120.30
1	1A	1441	G	O5'-P-OP1	5.27	117.03	110.70
32	2a	532	A	C2-N3-C4	5.27	113.24	110.60
1	1A	20	C	N3-C4-C5	5.27	124.01	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1627	G	C8-N9-C4	-5.27	104.29	106.40
1	1A	2035	G	N1-C6-O6	-5.27	116.74	119.90
2	2B	116	G	N7-C8-N9	-5.27	110.47	113.10
1	1A	146	G	C8-N9-C4	5.27	108.51	106.40
1	1A	271(S)	G	N1-C6-O6	5.27	123.06	119.90
1	2A	219	G	C8-N9-C4	-5.27	104.29	106.40
1	2A	1804	C	C4-C5-C6	-5.27	114.77	117.40
32	2a	1120	G	N3-C4-C5	5.27	131.24	128.60
1	1A	269	U	N1-C2-N3	-5.27	111.74	114.90
1	1A	765	G	C5-C6-N1	-5.27	108.87	111.50
1	1A	776	G	C6-N1-C2	-5.27	121.94	125.10
1	1A	1031	G	C6-C5-N7	-5.27	127.24	130.40
1	1A	1233	C	N3-C4-C5	5.27	124.01	121.90
1	1A	1554	A	N1-C2-N3	-5.27	126.67	129.30
1	1A	2166	G	N1-C6-O6	-5.27	116.74	119.90
1	1A	2261	C	C5-C4-N4	5.27	123.89	120.20
1	1A	2283	C	C6-N1-C2	5.27	122.41	120.30
1	1A	2578	G	C6-N1-C2	-5.27	121.94	125.10
1	1A	2663	G	N9-C4-C5	5.27	107.51	105.40
1	2A	1427	A	N1-C6-N6	-5.27	115.44	118.60
1	2A	1620	G	N3-C2-N2	-5.27	116.21	119.90
1	2A	1848	A	C5-C6-N1	5.27	120.33	117.70
1	2A	2267	A	OP1-P-O3'	5.27	116.79	105.20
1	1A	2883	A	N1-C6-N6	5.27	121.76	118.60
1	1A	2888	C	C5-C4-N4	5.27	123.89	120.20
32	1a	296	U	N3-C4-C5	-5.27	111.44	114.60
1	1A	194	G	C2-N3-C4	-5.26	109.27	111.90
1	1A	1641	A	C4-C5-N7	-5.26	108.07	110.70
1	1A	2657	A	C2-N3-C4	5.26	113.23	110.60
32	1a	559	A	O4'-C1'-N9	5.26	112.41	108.20
32	1a	734	G	N3-C2-N2	5.26	123.58	119.90
1	2A	946	G	C5-C6-N1	-5.26	108.87	111.50
1	2A	2674	G	C5-C6-O6	-5.26	125.44	128.60
3	2D	229	VAL	CB-CA-C	-5.26	101.40	111.40
4	2E	144	ARG	NE-CZ-NH2	-5.26	117.67	120.30
32	2a	230	G	N3-C4-C5	-5.26	125.97	128.60
32	2a	893	C	C5-C4-N4	-5.26	116.51	120.20
32	1a	351	G	OP2-P-O3'	5.26	116.78	105.20
1	2A	1204	A	C8-N9-C4	5.26	107.91	105.80
1	1A	1300	U	N3-C2-O2	-5.26	118.52	122.20
1	1A	1459	G	N1-C6-O6	5.26	123.06	119.90
1	1A	1693	U	O4'-C1'-N1	-5.26	103.99	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2447	G	N9-C1'-C2'	5.26	120.84	114.00
32	1a	177	C	O5'-P-OP1	-5.26	100.96	105.70
1	2A	226	G	N1-C2-N2	5.26	120.93	116.20
1	2A	452	G	C6-N1-C2	-5.26	121.94	125.10
1	2A	743	G	C5-C6-N1	5.26	114.13	111.50
1	2A	1289	C	N1-C2-O2	-5.26	115.74	118.90
1	2A	1660	C	C2-N1-C1'	-5.26	113.01	118.80
1	2A	1809	A	O5'-P-OP2	5.26	117.01	110.70
1	2A	1899	G	O5'-P-OP2	-5.26	100.96	105.70
1	2A	2060	A	OP1-P-O3'	5.26	116.77	105.20
2	2B	68	C	C6-N1-C2	5.26	122.41	120.30
32	2a	251	G	C8-N9-C4	5.26	108.50	106.40
1	1A	271(W)	G	C2-N3-C4	-5.26	109.27	111.90
1	1A	563	G	C6-C5-N7	5.26	133.56	130.40
1	1A	968	G	C8-N9-C4	-5.26	104.30	106.40
1	1A	1364	G	C5-C6-O6	5.26	131.76	128.60
1	1A	1823	G	N3-C2-N2	5.26	123.58	119.90
1	1A	1883	G	O5'-P-OP2	-5.26	100.97	105.70
1	1A	1954	G	C6-C5-N7	-5.26	127.24	130.40
1	1A	2773	C	N3-C4-C5	-5.26	119.80	121.90
1	1A	2834	G	C5-N7-C8	5.26	106.93	104.30
1	2A	1554	A	N9-C4-C5	5.26	107.90	105.80
1	2A	1968	G	N3-C4-C5	5.26	131.23	128.60
1	2A	2070	G	C5-C6-N1	5.26	114.13	111.50
32	2a	1134	G	C8-N9-C4	-5.26	104.30	106.40
1	1A	1662	C	OP2-P-O3'	5.26	116.77	105.20
1	1A	2071	A	C2-N3-C4	-5.26	107.97	110.60
32	1a	551	U	C5-C6-N1	-5.26	120.07	122.70
1	2A	1577	C	C6-N1-C2	5.26	122.40	120.30
32	2a	163	C	C2-N1-C1'	5.26	124.58	118.80
1	1A	824	A	C5-N7-C8	-5.26	101.27	103.90
1	1A	1573	G	N7-C8-N9	-5.26	110.47	113.10
32	1a	156	G	C8-N9-C4	-5.26	104.30	106.40
32	1a	300	A	C6-C5-N7	-5.26	128.62	132.30
1	2A	468	G	C8-N9-C4	5.26	108.50	106.40
1	2A	593	G	C4-C5-N7	5.26	112.90	110.80
1	2A	2018	G	N1-C6-O6	5.26	123.05	119.90
12	2Q	16	ARG	NE-CZ-NH1	-5.26	117.67	120.30
32	2a	233	C	C6-N1-C2	-5.26	118.20	120.30
32	2a	481	G	N3-C4-N9	5.26	129.15	126.00
1	1A	306	U	N1-C2-N3	5.25	118.05	114.90
1	1A	1132	A	C8-N9-C4	-5.25	103.70	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1616	A	C8-N9-C4	-5.25	103.70	105.80
1	1A	2069	G	N3-C4-C5	-5.25	125.97	128.60
32	1a	1422	G	OP1-P-OP2	5.25	127.48	119.60
1	2A	1016	G	N7-C8-N9	-5.25	110.47	113.10
1	2A	1649	G	C4-N9-C1'	5.25	133.33	126.50
1	2A	1675	C	O5'-P-OP2	5.25	117.01	110.70
32	2a	1484	C	N3-C2-O2	5.25	125.58	121.90
1	1A	459	U	O5'-P-OP1	5.25	117.00	110.70
1	1A	508	G	C8-N9-C4	5.25	108.50	106.40
1	1A	1187	G	N7-C8-N9	5.25	115.73	113.10
1	1A	2112	G	N7-C8-N9	5.25	115.73	113.10
1	1A	2494	G	C5-C6-O6	5.25	131.75	128.60
32	1a	15	G	O5'-P-OP2	-5.25	100.97	105.70
32	1a	397	A	C4-N9-C1'	5.25	135.76	126.30
1	2A	123	G	C2-N3-C4	-5.25	109.27	111.90
1	2A	207	A	C5-C6-N1	-5.25	115.07	117.70
1	2A	797	C	C2-N3-C4	5.25	122.53	119.90
1	2A	2323	G	C2-N3-C4	-5.25	109.27	111.90
1	2A	2427	C	O5'-P-OP2	5.25	117.00	110.70
1	1A	1020	A	N1-C6-N6	-5.25	115.45	118.60
1	1A	2399	G	C4-C5-N7	-5.25	108.70	110.80
2	1B	102	A	N9-C4-C5	-5.25	103.70	105.80
1	2A	208	C	C6-N1-C2	5.25	122.40	120.30
1	2A	568	U	C5-C4-O4	-5.25	122.75	125.90
1	2A	851	U	N1-C2-N3	5.25	118.05	114.90
1	2A	2079	U	C4-C5-C6	5.25	122.85	119.70
1	2A	2594	C	N1-C2-O2	-5.25	115.75	118.90
1	1A	362	U	N3-C2-O2	5.25	125.88	122.20
1	1A	508	G	C8-N9-C1'	5.25	133.82	127.00
1	1A	571	A	N1-C2-N3	-5.25	126.67	129.30
1	1A	685	A	N7-C8-N9	5.25	116.42	113.80
1	1A	848	G	C5-C6-O6	-5.25	125.45	128.60
1	1A	2437	U	N1-C2-N3	5.25	118.05	114.90
1	1A	194	G	N1-C6-O6	5.25	123.05	119.90
1	1A	320	A	N1-C6-N6	5.25	121.75	118.60
1	1A	879	G	C8-N9-C4	-5.25	104.30	106.40
1	1A	1158	C	C2-N3-C4	-5.25	117.28	119.90
1	1A	1466	G	N1-C2-N2	5.25	120.92	116.20
1	1A	1490	A	C8-N9-C4	5.25	107.90	105.80
1	1A	1754	C	N1-C2-O2	5.25	122.05	118.90
1	1A	2407	G	N1-C2-N3	5.25	127.05	123.90
1	2A	506	G	C6-C5-N7	-5.25	127.25	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1537	G	N3-C4-N9	5.25	129.15	126.00
1	2A	1845	G	N1-C6-O6	-5.25	116.75	119.90
1	2A	2522	U	O5'-P-OP2	-5.25	100.98	105.70
24	22	3	LEU	CA-CB-CG	-5.25	103.23	115.30
1	1A	117	G	N7-C8-N9	-5.25	110.48	113.10
1	1A	990	A	OP1-P-OP2	-5.25	111.73	119.60
1	1A	2393	A	C5-C6-N6	5.25	127.90	123.70
1	1A	2500	U	O4'-C1'-N1	5.25	112.40	108.20
32	1a	127	G	N1-C6-O6	5.25	123.05	119.90
32	1a	187	C	C6-N1-C1'	-5.25	114.50	120.80
32	1a	758	G	C4-C5-N7	5.25	112.90	110.80
1	2A	43	A	N1-C6-N6	5.25	121.75	118.60
1	2A	988	A	N7-C8-N9	5.25	116.42	113.80
1	2A	1243	G	N1-C6-O6	5.25	123.05	119.90
1	2A	1496	A	N7-C8-N9	5.25	116.42	113.80
1	2A	1626	G	OP1-P-O3'	5.25	116.74	105.20
1	2A	2735	G	C2-N3-C4	5.25	114.52	111.90
1	1A	32	C	N3-C4-N4	5.25	121.67	118.00
1	1A	88	G	C2-N3-C4	-5.25	109.28	111.90
1	1A	2315	G	C5-C6-O6	-5.25	125.45	128.60
32	1a	1481	U	N3-C4-C5	-5.25	111.45	114.60
1	2A	774	A	C4-C5-C6	5.25	119.62	117.00
1	2A	964	C	C5-C6-N1	5.25	123.62	121.00
1	2A	1748	G	C5-C6-N1	-5.25	108.88	111.50
32	2a	346	G	N1-C6-O6	-5.25	116.75	119.90
1	1A	19	C	C4-C5-C6	5.24	120.02	117.40
1	1A	1645	G	N1-C6-O6	-5.24	116.75	119.90
1	1A	2594	C	N3-C4-C5	-5.24	119.80	121.90
32	1a	1370	G	C4-C5-N7	5.24	112.90	110.80
1	2A	327	G	C6-C5-N7	5.24	133.55	130.40
32	2a	1095	U	C5-C6-N1	-5.24	120.08	122.70
1	1A	1564	C	C5-C4-N4	5.24	123.87	120.20
32	1a	922	G	C6-C5-N7	-5.24	127.25	130.40
32	1a	1531	A	N1-C2-N3	-5.24	126.68	129.30
1	2A	129	C	C5-C6-N1	-5.24	118.38	121.00
1	2A	1264	G	C2-N3-C4	-5.24	109.28	111.90
1	1A	81	G	C8-N9-C4	5.24	108.50	106.40
1	1A	852	G	N9-C4-C5	5.24	107.50	105.40
1	1A	1509	C	C6-N1-C2	-5.24	118.20	120.30
1	1A	1520	G	C6-C5-N7	5.24	133.54	130.40
1	1A	1597	A	O5'-P-OP1	5.24	116.99	110.70
1	1A	2453	A	O5'-P-OP1	-5.24	100.98	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2505	G	C6-C5-N7	-5.24	127.25	130.40
1	1A	2699	C	C5-C4-N4	-5.24	116.53	120.20
2	1B	43	C	C6-N1-C2	-5.24	118.20	120.30
2	1B	113	G	N9-C4-C5	-5.24	103.30	105.40
32	1a	397	A	C4-C5-C6	5.24	119.62	117.00
32	1a	721	G	C4-N9-C1'	5.24	133.31	126.50
32	1a	1321	C	C5-C6-N1	5.24	123.62	121.00
1	2A	677	A	C5-C6-N1	5.24	120.32	117.70
1	2A	777	A	C8-N9-C4	-5.24	103.70	105.80
1	2A	800	A	C6-N1-C2	5.24	121.74	118.60
1	2A	833	U	C6-N1-C2	-5.24	117.86	121.00
1	2A	975(A)	G	C8-N9-C4	-5.24	104.30	106.40
32	2a	1059	C	C6-N1-C2	-5.24	118.20	120.30
32	2a	1391	U	C2-N1-C1'	-5.24	111.41	117.70
1	1A	827	U	N1-C2-O2	-5.24	119.13	122.80
1	1A	1218	C	C2-N3-C4	5.24	122.52	119.90
1	1A	1284	A	O5'-P-OP2	-5.24	100.98	105.70
1	1A	1786	A	O5'-P-OP2	-5.24	100.98	105.70
1	1A	1997	G	N7-C8-N9	5.24	115.72	113.10
1	1A	2826	A	N9-C4-C5	-5.24	103.70	105.80
32	1a	43	C	C6-N1-C2	5.24	122.40	120.30
32	1a	107	G	C8-N9-C4	5.24	108.50	106.40
1	2A	2789	C	N3-C4-N4	-5.24	114.33	118.00
32	2a	129	U	N3-C4-C5	-5.24	111.46	114.60
32	2a	1465	C	C6-N1-C1'	-5.24	114.51	120.80
1	1A	1164	G	C5-N7-C8	5.24	106.92	104.30
1	1A	2278	A	C8-N9-C4	5.24	107.89	105.80
32	1a	915	A	N1-C6-N6	-5.24	115.46	118.60
1	2A	2538	C	N3-C4-N4	-5.24	114.33	118.00
1	2A	2754	U	OP2-P-O3'	5.24	116.72	105.20
32	2a	453	A	N3-C4-C5	-5.24	123.13	126.80
1	1A	27	G	C4-C5-N7	5.24	112.89	110.80
1	1A	1412	A	C8-N9-C4	-5.24	103.71	105.80
1	1A	2331	G	C8-N9-C1'	-5.24	120.19	127.00
1	1A	2516	G	N1-C6-O6	5.24	123.04	119.90
2	1B	110	G	C8-N9-C4	-5.24	104.31	106.40
1	2A	787	U	C6-N1-C2	-5.24	117.86	121.00
1	2A	2781	A	C8-N9-C4	-5.24	103.71	105.80
1	1A	146	G	N9-C4-C5	-5.23	103.31	105.40
1	1A	191	A	N9-C4-C5	5.23	107.89	105.80
1	1A	2234	G	C8-N9-C4	5.23	108.49	106.40
2	1B	91	C	O5'-P-OP2	-5.23	100.99	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	190	A	C8-N9-C4	5.23	107.89	105.80
1	2A	805	G	N3-C4-C5	-5.23	125.98	128.60
1	2A	1566	A	C6-N1-C2	-5.23	115.46	118.60
1	1A	1239	G	C2-N3-C4	-5.23	109.28	111.90
1	1A	1834	U	C5-C4-O4	-5.23	122.76	125.90
1	1A	2307	G	N1-C6-O6	5.23	123.04	119.90
1	1A	2371	G	C5-N7-C8	5.23	106.92	104.30
32	1a	286	G	N3-C4-N9	-5.23	122.86	126.00
32	1a	1058	G	N7-C8-N9	-5.23	110.48	113.10
1	2A	95	G	C5-C6-O6	-5.23	125.46	128.60
1	2A	371	A	C4-C5-N7	5.23	113.32	110.70
1	2A	1280	G	O5'-P-OP1	5.23	116.98	110.70
1	2A	1285	G	C6-C5-N7	-5.23	127.26	130.40
1	2A	1405	U	C5-C6-N1	-5.23	120.08	122.70
1	2A	1985	G	O5'-P-OP2	-5.23	100.99	105.70
32	2a	1016	A	N9-C4-C5	-5.23	103.71	105.80
32	2a	1507	A	N9-C4-C5	-5.23	103.71	105.80
1	1A	987	G	C6-N1-C2	-5.23	121.96	125.10
1	1A	1471	A	OP1-P-OP2	-5.23	111.75	119.60
1	1A	2081	C	O5'-P-OP2	-5.23	100.99	105.70
1	1A	2421	G	C8-N9-C4	5.23	108.49	106.40
1	1A	2748	A	N9-C4-C5	-5.23	103.71	105.80
32	1a	189(L)	G	OP1-P-O3'	5.23	116.71	105.20
32	2a	1156	G	N3-C4-C5	-5.23	125.98	128.60
1	1A	906	G	N7-C8-N9	5.23	115.71	113.10
1	1A	2088	G	N9-C4-C5	-5.23	103.31	105.40
32	1a	1480	G	N3-C4-N9	-5.23	122.86	126.00
1	2A	1075	C	C5-C6-N1	5.23	123.61	121.00
3	2D	218	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	1A	245	G	C8-N9-C4	5.23	108.49	106.40
1	1A	541	C	O5'-P-OP2	-5.23	100.99	105.70
1	1A	1616	A	N7-C8-N9	5.23	116.41	113.80
1	1A	1900	A	C5-C6-N1	5.23	120.31	117.70
1	1A	2778	A	N1-C2-N3	5.23	131.91	129.30
2	1B	69	G	O5'-P-OP1	5.23	116.97	110.70
1	2A	123	G	OP1-P-OP2	5.23	127.44	119.60
1	2A	214	G	N3-C2-N2	5.23	123.56	119.90
1	2A	2297	C	C6-N1-C2	5.23	122.39	120.30
1	1A	1368	G	C4-N9-C1'	5.23	133.29	126.50
1	1A	1674	G	C8-N9-C1'	-5.23	120.21	127.00
32	1a	882	C	N3-C4-N4	5.23	121.66	118.00
1	2A	658	C	O5'-P-OP2	-5.23	101.00	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1220	A	C5-C6-N6	-5.23	119.52	123.70
1	2A	1955	U	C2-N3-C4	-5.23	123.86	127.00
1	2A	2237	G	C4-C5-N7	-5.23	108.71	110.80
1	1A	83	G	C2-N3-C4	-5.22	109.29	111.90
1	1A	620	G	N9-C4-C5	-5.22	103.31	105.40
1	1A	1022	G	OP1-P-O3'	5.22	116.69	105.20
1	1A	2464	C	N3-C4-N4	5.22	121.66	118.00
1	1A	2509	G	C4-C5-C6	-5.22	115.67	118.80
2	1B	77	U	OP2-P-O3'	5.22	116.69	105.20
1	2A	139	G	N1-C6-O6	5.22	123.03	119.90
1	2A	1646	C	N1-C2-O2	5.22	122.03	118.90
1	2A	1689	A	C4-C5-N7	5.22	113.31	110.70
1	2A	1690	A	N7-C8-N9	-5.22	111.19	113.80
32	2a	626	U	C6-N1-C2	5.22	124.13	121.00
32	2a	726	C	OP1-P-OP2	5.22	127.44	119.60
32	2a	814	A	O5'-P-OP2	-5.22	101.00	105.70
1	1A	251	A	C5-C6-N1	5.22	120.31	117.70
1	1A	674	G	C6-C5-N7	-5.22	127.27	130.40
1	1A	1440	G	C5-N7-C8	5.22	106.91	104.30
1	1A	1447	G	C8-N9-C4	-5.22	104.31	106.40
1	1A	2043	C	C2-N3-C4	5.22	122.51	119.90
1	2A	66	C	C6-N1-C2	-5.22	118.21	120.30
1	2A	755	C	C5-C4-N4	-5.22	116.54	120.20
1	2A	1820	U	C6-N1-C2	5.22	124.13	121.00
32	2a	299	G	C4-C5-N7	5.22	112.89	110.80
1	1A	1966	A	N1-C2-N3	-5.22	126.69	129.30
15	1T	9	LEU	CB-CG-CD2	5.22	119.88	111.00
32	1a	880	C	N3-C2-O2	5.22	125.55	121.90
1	2A	2544	G	OP1-P-OP2	-5.22	111.77	119.60
1	1A	783	A	N9-C4-C5	5.22	107.89	105.80
1	1A	878	A	N1-C2-N3	5.22	131.91	129.30
1	1A	940	G	C5-C6-O6	-5.22	125.47	128.60
1	1A	2354	G	C5-C6-N1	-5.22	108.89	111.50
1	1A	2690	C	N3-C2-O2	5.22	125.55	121.90
32	1a	1265	G	N1-C6-O6	5.22	123.03	119.90
32	1a	1351	U	C6-N1-C2	-5.22	117.87	121.00
1	2A	593	G	C2-N3-C4	-5.22	109.29	111.90
1	2A	1501	C	N1-C2-O2	-5.22	115.77	118.90
1	2A	2243	U	C6-N1-C2	5.22	124.13	121.00
1	2A	2583	G	C5-N7-C8	-5.22	101.69	104.30
1	1A	2378	A	C6-C5-N7	-5.22	128.65	132.30
32	1a	1516	G	N3-C2-N2	-5.22	116.25	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	272	G	C4-C5-N7	5.22	112.89	110.80
32	2a	721	G	C8-N9-C1'	-5.22	120.22	127.00
1	1A	1342	A	O4'-C1'-N9	-5.22	104.03	108.20
1	1A	1762	A	N1-C6-N6	-5.22	115.47	118.60
1	1A	1893	C	O5'-P-OP2	-5.22	101.01	105.70
1	1A	2148	G	C4-N9-C1'	-5.22	119.72	126.50
1	1A	2227	A	N9-C4-C5	5.22	107.89	105.80
1	1A	2377	A	C8-N9-C4	5.22	107.89	105.80
1	1A	2562	U	N3-C4-C5	-5.22	111.47	114.60
1	1A	2599	G	C6-C5-N7	5.22	133.53	130.40
32	1a	926	G	C5-N7-C8	-5.22	101.69	104.30
32	1a	1084	G	C6-C5-N7	-5.22	127.27	130.40
1	2A	450	G	C5-C6-O6	5.22	131.73	128.60
1	2A	555	U	C5-C4-O4	5.22	129.03	125.90
1	1A	73	A	N1-C6-N6	-5.21	115.47	118.60
1	1A	2035	G	O4'-C1'-N9	5.21	112.37	108.20
32	1a	595	G	N3-C4-C5	-5.21	125.99	128.60
32	1a	753	A	O4'-C1'-N9	-5.21	104.03	108.20
1	2A	789	A	N1-C2-N3	-5.21	126.69	129.30
1	2A	1132	A	C2-N3-C4	5.21	113.21	110.60
1	2A	1314	C	C6-N1-C2	-5.21	118.21	120.30
1	2A	1772	G	C4-N9-C1'	-5.21	119.72	126.50
32	2a	1394	A	N1-C6-N6	5.21	121.73	118.60
1	1A	1349	A	C8-N9-C4	5.21	107.89	105.80
1	1A	1368	G	N3-C4-N9	5.21	129.13	126.00
1	1A	1410	G	N3-C4-N9	-5.21	122.87	126.00
1	1A	2102	U	C5-C6-N1	5.21	125.31	122.70
1	2A	384	U	N3-C2-O2	-5.21	118.55	122.20
1	2A	683	C	O5'-P-OP2	5.21	116.95	110.70
1	2A	1931	U	OP1-P-OP2	-5.21	111.78	119.60
1	2A	2617	C	N3-C4-N4	5.21	121.65	118.00
32	2a	689	C	C6-N1-C2	-5.21	118.22	120.30
32	2a	1488	G	C8-N9-C4	-5.21	104.31	106.40
1	1A	198	C	C2-N1-C1'	5.21	124.53	118.80
1	1A	710	G	N1-C6-O6	5.21	123.03	119.90
1	1A	1295	C	N3-C4-C5	5.21	123.98	121.90
1	1A	1399	C	OP2-P-O3'	5.21	116.67	105.20
1	1A	1598	C	O5'-P-OP2	5.21	116.95	110.70
1	1A	2024	G	N9-C4-C5	-5.21	103.31	105.40
1	1A	2507	C	C5-C6-N1	5.21	123.61	121.00
1	1A	2894	G	C8-N9-C1'	5.21	133.78	127.00
2	1B	80	U	C5-C4-O4	5.21	129.03	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	329	A	C4-C5-C6	5.21	119.61	117.00
32	1a	964	A	N7-C8-N9	-5.21	111.19	113.80
32	1a	1525	G	N1-C6-O6	5.21	123.03	119.90
1	2A	1490	A	O5'-P-OP2	5.21	116.95	110.70
1	2A	1891	G	C4-N9-C1'	-5.21	119.72	126.50
1	2A	2677	G	C4-C5-N7	5.21	112.88	110.80
1	2A	2721	A	O5'-P-OP2	5.21	116.95	110.70
32	2a	357	G	C8-N9-C4	-5.21	104.32	106.40
1	1A	136	G	N9-C4-C5	-5.21	103.32	105.40
1	1A	841	A	P-O3'-C3'	-5.21	113.45	119.70
1	1A	1966	A	N7-C8-N9	-5.21	111.19	113.80
1	2A	2183	C	C6-N1-C1'	5.21	127.05	120.80
1	2A	2351	G	C6-C5-N7	-5.21	127.27	130.40
1	1A	2717	G	C4-C5-N7	5.21	112.88	110.80
1	1A	2871	C	O5'-P-OP1	5.21	116.95	110.70
32	1a	343	U	N1-C1'-C2'	-5.21	106.27	112.00
32	1a	423	G	C5-C6-O6	-5.21	125.47	128.60
32	1a	1082	G	N1-C6-O6	5.21	123.03	119.90
32	2a	397	A	C4-N9-C1'	5.21	135.67	126.30
32	2a	905	U	C6-N1-C2	-5.21	117.88	121.00
32	2a	1034	G	N3-C2-N2	-5.21	116.25	119.90
1	1A	792	G	C8-N9-C1'	-5.21	120.23	127.00
1	1A	2032	G	N9-C4-C5	-5.21	103.32	105.40
1	1A	2073	C	N3-C2-O2	5.21	125.54	121.90
1	1A	2315	G	OP1-P-O3'	5.21	116.65	105.20
32	1a	122	G	C8-N9-C4	5.21	108.48	106.40
32	1a	737	A	C5-N7-C8	-5.21	101.30	103.90
1	2A	205	G	N3-C2-N2	5.21	123.55	119.90
1	2A	2640	G	C4-C5-N7	-5.21	108.72	110.80
1	2A	2818	G	N3-C4-N9	-5.21	122.88	126.00
32	2a	362	G	N3-C4-N9	-5.21	122.88	126.00
32	2a	1274	G	N1-C6-O6	5.21	123.02	119.90
1	1A	245	G	OP1-P-O3'	5.21	116.65	105.20
1	1A	2538	C	OP1-P-OP2	5.21	127.41	119.60
32	1a	880	C	C6-N1-C2	5.21	122.38	120.30
1	2A	1023	U	C2-N1-C1'	-5.21	111.45	117.70
1	1A	148	C	C2-N1-C1'	-5.20	113.08	118.80
1	1A	1082	U	C3'-C2'-C1'	-5.20	97.34	101.50
1	1A	1549	C	O5'-P-OP1	-5.20	101.02	105.70
32	1a	362	G	C8-N9-C4	-5.20	104.32	106.40
1	2A	206	U	C5-C6-N1	5.20	125.30	122.70
1	2A	657	U	C5-C6-N1	-5.20	120.10	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	682	G	C8-N9-C1'	-5.20	120.23	127.00
1	2A	1063	G	C8-N9-C4	-5.20	104.32	106.40
1	2A	2506	U	C2-N3-C4	-5.20	123.88	127.00
32	2a	41	G	C5-C6-N1	-5.20	108.90	111.50
1	1A	1994	C	O5'-P-OP1	5.20	116.94	110.70
1	1A	2182	G	C8-N9-C4	-5.20	104.32	106.40
1	2A	26	G	N9-C4-C5	-5.20	103.32	105.40
1	2A	1142	U	C5-C4-O4	5.20	129.02	125.90
1	2A	1216	G	N3-C4-C5	-5.20	126.00	128.60
1	2A	1461	G	N1-C6-O6	-5.20	116.78	119.90
1	2A	2413	G	N9-C4-C5	-5.20	103.32	105.40
25	23	18	ASP	CB-CG-OD1	5.20	122.98	118.30
32	2a	562	C	C6-N1-C2	5.20	122.38	120.30
1	1A	391	G	C4-C5-N7	5.20	112.88	110.80
1	1A	1214	A	C5-C6-N6	-5.20	119.54	123.70
1	1A	1579	A	C5-N7-C8	-5.20	101.30	103.90
1	1A	2487	G	C8-N9-C4	5.20	108.48	106.40
1	1A	2817	G	N9-C4-C5	5.20	107.48	105.40
1	2A	706	A	C8-N9-C4	5.20	107.88	105.80
1	2A	959	A	N3-C4-N9	5.20	131.56	127.40
1	2A	2250	G	OP1-P-OP2	5.20	127.40	119.60
1	1A	192	C	OP1-P-O3'	5.20	116.64	105.20
1	1A	206	U	C2-N1-C1'	-5.20	111.46	117.70
1	1A	1147	C	O5'-P-OP1	5.20	116.94	110.70
1	1A	1192	G	C8-N9-C4	5.20	108.48	106.40
1	1A	1967	C	N3-C2-O2	-5.20	118.26	121.90
1	2A	792	G	C5-C6-N1	5.20	114.10	111.50
1	2A	1317	A	C8-N9-C4	5.20	107.88	105.80
1	2A	1707	G	C8-N9-C4	5.20	108.48	106.40
1	2A	1998	G	C2-N3-C4	-5.20	109.30	111.90
1	2A	2838	G	N1-C6-O6	5.20	123.02	119.90
1	1A	1228	G	C5-C6-O6	-5.20	125.48	128.60
1	2A	1937	A	C5-N7-C8	5.20	106.50	103.90
1	2A	2321	G	N3-C4-N9	5.20	129.12	126.00
1	1A	54	G	C6-C5-N7	-5.20	127.28	130.40
1	1A	944	G	C5-C6-N1	-5.20	108.90	111.50
1	1A	1240	U	N3-C4-C5	-5.20	111.48	114.60
1	1A	1479	G	N3-C2-N2	-5.20	116.26	119.90
1	1A	2085	C	C4-C5-C6	5.20	120.00	117.40
1	1A	2655	G	OP2-P-O3'	5.20	116.63	105.20
32	1a	219	C	C5-C6-N1	5.20	123.60	121.00
32	1a	241	C	C6-N1-C2	-5.20	118.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	770	C	OP1-P-OP2	-5.20	111.81	119.60
1	2A	648	G	C8-N9-C4	-5.20	104.32	106.40
1	2A	1202	C	C4-C5-C6	5.20	120.00	117.40
1	2A	2560	C	N3-C2-O2	5.20	125.54	121.90
1	2A	2805	G	O4'-C1'-N9	5.20	112.36	108.20
1	1A	29	U	C6-N1-C2	-5.19	117.88	121.00
1	1A	2425	A	O5'-P-OP2	-5.19	101.03	105.70
32	1a	37	U	C5-C6-N1	-5.19	120.10	122.70
32	1a	568	G	O5'-P-OP1	-5.19	101.03	105.70
1	2A	298	G	C5-C6-O6	-5.19	125.48	128.60
1	2A	327	G	C8-N9-C4	5.19	108.48	106.40
1	2A	837	C	C6-N1-C2	-5.19	118.22	120.30
32	2a	393	A	OP1-P-O3'	5.19	116.63	105.20
1	1A	394	A	C6-N1-C2	-5.19	115.48	118.60
1	1A	1147	C	C6-N1-C2	5.19	122.38	120.30
1	1A	1257	C	C5-C4-N4	5.19	123.83	120.20
1	1A	2417	C	N3-C2-O2	-5.19	118.27	121.90
1	1A	2659	G	N3-C4-C5	5.19	131.20	128.60
1	1A	2767	C	C4-C5-C6	5.19	120.00	117.40
1	2A	1190	G	C6-N1-C2	-5.19	121.98	125.10
1	2A	1679	U	OP2-P-O3'	5.19	116.62	105.20
1	2A	2056	G	N3-C2-N2	-5.19	116.27	119.90
2	2B	98	G	C5-C6-O6	5.19	131.72	128.60
32	2a	481	G	N3-C4-C5	-5.19	126.00	128.60
1	1A	95	G	C4-C5-C6	5.19	121.91	118.80
1	1A	473	G	C8-N9-C4	5.19	108.48	106.40
1	1A	1418	G	C5-C6-O6	5.19	131.72	128.60
1	1A	2284	C	OP1-P-OP2	5.19	127.39	119.60
1	1A	2725	A	N1-C2-N3	5.19	131.90	129.30
1	1A	2740	A	N3-C4-C5	-5.19	123.17	126.80
13	1R	45	ARG	NE-CZ-NH1	5.19	122.90	120.30
32	1a	15	G	C8-N9-C1'	-5.19	120.25	127.00
1	2A	150	C	C2-N1-C1'	-5.19	113.09	118.80
1	2A	794	G	N3-C4-C5	5.19	131.20	128.60
1	2A	2729	G	C2-N3-C4	-5.19	109.31	111.90
1	2A	2738	A	C5-C6-N6	5.19	127.85	123.70
32	2a	115	G	N3-C4-C5	-5.19	126.00	128.60
32	2a	446	G	N7-C8-N9	5.19	115.69	113.10
32	2a	753	A	N1-C2-N3	5.19	131.90	129.30
32	1a	235	C	OP1-P-OP2	5.19	127.38	119.60
32	1a	321	A	N7-C8-N9	-5.19	111.21	113.80
32	1a	807	A	N1-C6-N6	-5.19	115.49	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1036	G	C8-N9-C4	5.19	108.48	106.40
1	2A	1653	G	C4-N9-C1'	5.19	133.25	126.50
1	2A	2061	G	C2-N3-C4	-5.19	109.31	111.90
1	2A	2362	G	OP1-P-OP2	5.19	127.38	119.60
1	1A	345	A	N7-C8-N9	5.19	116.39	113.80
1	1A	494	G	N7-C8-N9	5.19	115.69	113.10
1	1A	990	A	C4-C5-N7	5.19	113.29	110.70
1	1A	2494	G	C5-N7-C8	5.19	106.89	104.30
1	1A	2515	C	OP1-P-OP2	-5.19	111.82	119.60
1	1A	2526	G	C8-N9-C4	5.19	108.47	106.40
22	10	44	ARG	NE-CZ-NH1	-5.19	117.71	120.30
32	1a	150	C	C2-N3-C4	5.19	122.49	119.90
1	2A	859	G	N1-C6-O6	5.19	123.01	119.90
1	2A	2182	G	N1-C6-O6	-5.19	116.79	119.90
1	1A	826	U	N1-C2-N3	5.19	118.01	114.90
1	1A	919	G	OP2-P-O3'	5.19	116.61	105.20
1	1A	2537	U	OP1-P-OP2	5.19	127.38	119.60
2	1B	103	G	N3-C4-C5	5.19	131.19	128.60
13	1R	96	ARG	NE-CZ-NH1	-5.19	117.71	120.30
32	1a	1266	G	C8-N9-C4	-5.19	104.33	106.40
32	2a	117	G	C8-N9-C4	5.19	108.47	106.40
1	1A	597	U	N1-C2-O2	-5.18	119.17	122.80
1	1A	2116	G	N7-C8-N9	5.18	115.69	113.10
1	1A	2415	G	N3-C2-N2	-5.18	116.27	119.90
1	1A	2556	C	C6-N1-C2	5.18	122.37	120.30
1	1A	2780	G	N1-C6-O6	-5.18	116.79	119.90
32	1a	280	C	C5-C4-N4	-5.18	116.57	120.20
32	1a	289	G	C5-C6-N1	-5.18	108.91	111.50
32	1a	903	G	C2-N3-C4	-5.18	109.31	111.90
1	2A	457	A	N9-C4-C5	5.18	107.87	105.80
1	2A	1665	A	N1-C6-N6	-5.18	115.49	118.60
1	2A	2563	U	N3-C2-O2	-5.18	118.57	122.20
1	1A	27	G	OP1-P-O3'	5.18	116.60	105.20
1	1A	272	G	N3-C4-N9	5.18	129.11	126.00
1	1A	611	C	N3-C4-C5	5.18	123.97	121.90
1	1A	1634	A	C4-C5-N7	-5.18	108.11	110.70
1	1A	2003	G	C8-N9-C1'	-5.18	120.26	127.00
1	1A	2182	G	C5-C6-O6	5.18	131.71	128.60
1	1A	2255	G	N1-C6-O6	-5.18	116.79	119.90
2	1B	103	G	N3-C2-N2	-5.18	116.27	119.90
32	1a	960	U	C2-N1-C1'	5.18	123.92	117.70
32	1a	1105	A	C8-N9-C4	-5.18	103.73	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	936	C	N3-C2-O2	5.18	125.53	121.90
1	2A	2631	G	C8-N9-C4	-5.18	104.33	106.40
1	2A	2682	U	O5'-P-OP2	-5.18	101.04	105.70
1	2A	2739	U	C4-C5-C6	5.18	122.81	119.70
2	2B	103	G	N3-C4-C5	5.18	131.19	128.60
32	2a	1252	A	C5-C6-N6	5.18	127.85	123.70
1	1A	800	A	C4-C5-N7	-5.18	108.11	110.70
1	1A	1126	A	C2-N3-C4	-5.18	108.01	110.60
1	1A	2507	C	C6-N1-C2	-5.18	118.23	120.30
1	2A	299	A	N1-C6-N6	-5.18	115.49	118.60
1	2A	2589	A	N1-C6-N6	-5.18	115.49	118.60
1	1A	45	C	N1-C2-O2	-5.18	115.79	118.90
1	1A	529	A	N1-C2-N3	-5.18	126.71	129.30
1	1A	702	G	N1-C6-O6	5.18	123.01	119.90
1	1A	2643	G	C2-N3-C4	-5.18	109.31	111.90
32	1a	982	U	C6-N1-C2	5.18	124.11	121.00
1	2A	735	A	C4-C5-C6	5.18	119.59	117.00
1	2A	1314	C	C2-N1-C1'	5.18	124.50	118.80
1	2A	1601	G	C8-N9-C4	5.18	108.47	106.40
1	2A	1998	G	C8-N9-C4	5.18	108.47	106.40
1	2A	2015	A	OP2-P-O3'	5.18	116.60	105.20
1	1A	1561	G	C8-N9-C4	-5.18	104.33	106.40
32	1a	804	U	C5-C6-N1	-5.18	120.11	122.70
1	2A	62	C	C2-N1-C1'	-5.18	113.10	118.80
1	2A	1611	C	C5-C4-N4	-5.18	116.58	120.20
32	2a	7	G	C8-N9-C1'	5.18	133.73	127.00
32	2a	138	G	N1-C6-O6	5.18	123.01	119.90
32	2a	510	A	O5'-P-OP2	-5.18	101.04	105.70
32	2a	946	A	C5-C6-N1	-5.18	115.11	117.70
1	1A	1092	C	N1-C2-O2	5.18	122.01	118.90
1	1A	1195	G	C8-N9-C4	-5.18	104.33	106.40
1	1A	2319	G	C8-N9-C4	-5.18	104.33	106.40
32	1a	1341	U	C5-C6-N1	-5.18	120.11	122.70
1	2A	623	G	C2-N3-C4	5.18	114.49	111.90
1	2A	1273	U	C2-N3-C4	-5.18	123.89	127.00
1	2A	1967	C	C5-C6-N1	-5.18	118.41	121.00
1	2A	2011	U	N1-C2-O2	-5.18	119.18	122.80
1	2A	2242	G	O5'-P-OP1	5.18	116.91	110.70
32	2a	59	A	O4'-C1'-N9	-5.18	104.06	108.20
32	2a	364	A	O5'-P-OP1	5.18	116.91	110.70
1	1A	124	G	N1-C2-N3	5.17	127.00	123.90
1	1A	1368	G	C8-N9-C1'	-5.17	120.27	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1770	G	N7-C8-N9	-5.17	110.51	113.10
1	1A	1776	G	N1-C2-N2	-5.17	111.54	116.20
1	1A	2464	C	C5-C4-N4	-5.17	116.58	120.20
32	1a	878	G	C8-N9-C4	5.17	108.47	106.40
1	2A	452	G	C8-N9-C1'	-5.17	120.27	127.00
1	2A	584	C	N1-C2-O2	-5.17	115.80	118.90
1	2A	783	A	C5-C6-N6	5.17	127.84	123.70
1	2A	2598	A	C6-N1-C2	-5.17	115.50	118.60
1	2A	2718	G	C6-C5-N7	-5.17	127.30	130.40
8	2I	124	GLY	N-CA-C	5.17	126.04	113.10
32	2a	454	C	N3-C2-O2	-5.17	118.28	121.90
32	2a	946	A	N1-C2-N3	5.17	131.89	129.30
36	2e	12	LEU	CA-CB-CG	5.17	127.20	115.30
1	1A	781	A	P-O3'-C3'	5.17	125.91	119.70
1	1A	1280	G	C5-C6-N1	-5.17	108.91	111.50
1	1A	2747	G	C4-C5-N7	5.17	112.87	110.80
1	2A	1210	A	OP2-P-O3'	5.17	116.58	105.20
1	2A	1509(A)	A	O4'-C1'-N9	5.17	112.34	108.20
1	1A	228	A	C5-C6-N1	5.17	120.28	117.70
1	1A	641	C	N3-C4-C5	-5.17	119.83	121.90
1	1A	2011	U	N3-C4-O4	5.17	123.02	119.40
1	1A	2271	G	N3-C2-N2	5.17	123.52	119.90
1	1A	2426	A	N1-C2-N3	5.17	131.88	129.30
32	1a	481	G	C4-N9-C1'	5.17	133.22	126.50
32	1a	1525	G	C6-C5-N7	-5.17	127.30	130.40
1	2A	27	G	OP1-P-O3'	5.17	116.58	105.20
1	2A	377	C	C5-C6-N1	-5.17	118.41	121.00
1	2A	1070	A	O4'-C1'-N9	5.17	112.34	108.20
1	2A	1145	C	N3-C4-C5	-5.17	119.83	121.90
1	2A	1295	C	C6-N1-C2	-5.17	118.23	120.30
1	2A	1817	G	C2-N3-C4	5.17	114.48	111.90
2	2B	63	G	N7-C8-N9	-5.17	110.51	113.10
32	2a	546	G	C8-N9-C4	-5.17	104.33	106.40
1	1A	614	U	C5-C4-O4	5.17	129.00	125.90
1	1A	675	A	OP2-P-O3'	5.17	116.57	105.20
1	1A	2770	G	O5'-P-OP1	5.17	116.90	110.70
1	2A	228	A	N1-C6-N6	5.17	121.70	118.60
1	2A	2325	G	N7-C8-N9	5.17	115.69	113.10
32	2a	1410	G	C4-C5-N7	-5.17	108.73	110.80
32	2a	1505	G	N3-C4-N9	-5.17	122.90	126.00
1	1A	926	A	N1-C6-N6	5.17	121.70	118.60
1	1A	1105	U	N1-C2-N3	-5.17	111.80	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1152	C	N3-C2-O2	5.17	125.52	121.90
32	1a	319	G	C5-C6-N1	-5.17	108.92	111.50
1	2A	234	C	C6-N1-C2	-5.17	118.23	120.30
1	2A	831	G	O5'-P-OP2	5.17	116.90	110.70
1	2A	1913	A	N1-C6-N6	-5.17	115.50	118.60
1	2A	2389	G	OP1-P-OP2	-5.17	111.85	119.60
32	2a	779	C	N3-C4-C5	5.17	123.97	121.90
32	2a	913	A	O4'-C1'-N9	-5.17	104.06	108.20
32	2a	1201	A	C6-N1-C2	-5.17	115.50	118.60
32	2a	1356	G	N7-C8-N9	5.17	115.68	113.10
1	1A	126	A	C8-N9-C4	-5.17	103.73	105.80
1	1A	678	C	C2-N3-C4	-5.17	117.32	119.90
1	1A	1779	U	N3-C4-O4	5.17	123.02	119.40
32	1a	292	G	O5'-P-OP1	5.17	116.90	110.70
32	1a	689	C	C6-N1-C2	-5.17	118.23	120.30
1	2A	478	A	N1-C6-N6	5.17	121.70	118.60
1	2A	582	G	N3-C2-N2	-5.17	116.28	119.90
1	2A	2774	C	O5'-P-OP2	-5.17	101.05	105.70
32	2a	123	C	OP2-P-O3'	5.17	116.56	105.20
32	2a	834	C	O5'-P-OP2	-5.17	101.05	105.70
32	2a	1287	A	C5-C6-N6	5.17	127.83	123.70
1	1A	203	C	C2-N3-C4	-5.17	117.32	119.90
1	1A	1697	G	OP1-P-OP2	-5.17	111.85	119.60
1	2A	556	G	OP1-P-OP2	-5.17	111.85	119.60
32	2a	841	U	C6-N1-C2	-5.17	117.90	121.00
1	1A	340	A	N1-C6-N6	-5.16	115.50	118.60
1	1A	669	G	N9-C4-C5	-5.16	103.33	105.40
1	1A	849	A	N1-C6-N6	5.16	121.70	118.60
1	1A	1344	G	N7-C8-N9	5.16	115.68	113.10
1	1A	1475	G	N1-C6-O6	5.16	123.00	119.90
1	1A	2512	C	N3-C4-N4	5.16	121.61	118.00
1	1A	2566	A	OP1-P-O3'	5.16	116.56	105.20
1	1A	2691	C	OP1-P-OP2	-5.16	111.85	119.60
32	1a	1376	U	N3-C2-O2	-5.16	118.58	122.20
1	2A	248	G	N9-C4-C5	5.16	107.47	105.40
1	2A	1642	G	C4-C5-C6	-5.16	115.70	118.80
1	2A	1688	U	C5-C4-O4	5.16	129.00	125.90
1	2A	2063	C	OP2-P-O3'	5.16	116.56	105.20
1	1A	27	G	N3-C2-N2	5.16	123.51	119.90
32	1a	426	G	N1-C6-O6	5.16	123.00	119.90
1	2A	148	C	N1-C2-N3	-5.16	115.59	119.20
1	2A	655	A	O4'-C1'-N9	5.16	112.33	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2B	20	C	O5'-P-OP1	5.16	116.89	110.70
1	1A	37	C	N1-C2-O2	5.16	122.00	118.90
1	1A	670	A	OP1-P-O3'	5.16	116.55	105.20
1	1A	675	A	C5-N7-C8	5.16	106.48	103.90
1	1A	1189	A	N1-C6-N6	5.16	121.70	118.60
1	1A	1789	A	P-O3'-C3'	-5.16	113.51	119.70
1	1A	2685	G	N1-C6-O6	-5.16	116.80	119.90
32	1a	334	C	C6-N1-C2	-5.16	118.23	120.30
32	1a	343	U	C4-C5-C6	-5.16	116.60	119.70
32	1a	721	G	C6-C5-N7	-5.16	127.30	130.40
1	2A	509	C	C4-C5-C6	5.16	119.98	117.40
1	2A	658	C	C4-C5-C6	5.16	119.98	117.40
1	2A	1969	A	OP1-P-O3'	5.16	116.55	105.20
1	2A	2582	G	C4-N9-C1'	5.16	133.21	126.50
2	2B	118	G	C5-C6-O6	5.16	131.70	128.60
1	1A	261	G	C5-C6-O6	-5.16	125.50	128.60
1	1A	661	C	N1-C2-O2	5.16	122.00	118.90
1	1A	1299	G	C4-C5-N7	5.16	112.86	110.80
1	2A	1068	G	C2-N3-C4	5.16	114.48	111.90
32	2a	1472	U	C5-C6-N1	-5.16	120.12	122.70
38	2g	101	LEU	CA-CB-CG	-5.16	103.44	115.30
1	1A	336	C	N3-C4-C5	-5.16	119.84	121.90
1	1A	1963	U	OP1-P-O3'	5.16	116.54	105.20
32	1a	1287	A	N9-C4-C5	5.16	107.86	105.80
1	2A	398	G	OP2-P-O3'	5.16	116.55	105.20
1	2A	563	G	N1-C2-N3	5.16	126.99	123.90
1	1A	743	G	N9-C4-C5	5.16	107.46	105.40
1	1A	892	G	N3-C4-C5	5.16	131.18	128.60
1	1A	1198	U	C6-N1-C2	-5.16	117.91	121.00
1	1A	1475	G	N3-C2-N2	-5.16	116.29	119.90
1	1A	1770	G	O5'-P-OP2	5.16	116.89	110.70
1	1A	2224	G	C5-N7-C8	5.16	106.88	104.30
1	1A	2258	C	C6-N1-C1'	-5.16	114.61	120.80
1	1A	2288	A	O4'-C1'-N9	-5.16	104.08	108.20
2	1B	27	C	C5-C6-N1	-5.16	118.42	121.00
1	2A	736	C	C6-N1-C2	5.16	122.36	120.30
1	2A	2495	G	C5-C6-O6	-5.16	125.51	128.60
1	1A	1430	C	C5-C4-N4	5.15	123.81	120.20
1	1A	1683	C	C2-N3-C4	-5.15	117.32	119.90
1	1A	1695	G	C4-C5-N7	5.15	112.86	110.80
1	1A	2735	G	C5-C6-N1	-5.15	108.92	111.50
1	1A	2770	G	C2-N3-C4	5.15	114.48	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1403	C	N3-C4-N4	-5.15	114.39	118.00
1	2A	2588	G	N1-C6-O6	5.15	122.99	119.90
22	20	15	ASP	N-CA-C	-5.15	97.08	111.00
32	2a	577	G	C4-C5-N7	5.15	112.86	110.80
1	1A	570	G	C2-N3-C4	5.15	114.48	111.90
1	1A	1165	U	N3-C2-O2	-5.15	118.59	122.20
1	1A	1546	C	O5'-P-OP1	-5.15	101.06	105.70
1	1A	1570	A	N1-C6-N6	5.15	121.69	118.60
1	1A	2654	A	N9-C4-C5	-5.15	103.74	105.80
1	1A	2706	G	N1-C2-N3	5.15	126.99	123.90
1	2A	118	A	N1-C2-N3	-5.15	126.72	129.30
1	2A	145	G	N3-C4-C5	5.15	131.18	128.60
1	2A	704	G	N3-C4-N9	-5.15	122.91	126.00
32	2a	231	G	C6-C5-N7	-5.15	127.31	130.40
32	2a	483	C	N3-C2-O2	5.15	125.51	121.90
32	2a	1387	G	C8-N9-C4	5.15	108.46	106.40
1	1A	131	G	OP2-P-O3'	5.15	116.53	105.20
1	1A	978	G	C2-N3-C4	-5.15	109.33	111.90
1	1A	1573	G	C4-N9-C1'	-5.15	119.81	126.50
1	1A	2448	A	N1-C2-N3	5.15	131.88	129.30
32	1a	73	G	N1-C6-O6	-5.15	116.81	119.90
1	2A	640	C	OP1-P-O3'	5.15	116.53	105.20
1	2A	1768	U	N3-C2-O2	5.15	125.81	122.20
32	2a	903	G	N7-C8-N9	-5.15	110.53	113.10
32	2a	926	G	C8-N9-C1'	-5.15	120.30	127.00
1	1A	695	G	C8-N9-C4	5.15	108.46	106.40
32	1a	265	G	C4-C5-N7	-5.15	108.74	110.80
32	1a	1146	A	N9-C4-C5	-5.15	103.74	105.80
1	2A	2080	G	C8-N9-C1'	5.15	133.69	127.00
1	1A	271(L)	U	N1-C2-N3	-5.15	111.81	114.90
1	1A	826	U	C2-N3-C4	-5.15	123.91	127.00
1	1A	1480	G	N1-C6-O6	5.15	122.99	119.90
3	1D	242	ARG	NE-CZ-NH2	-5.15	117.73	120.30
32	1a	735	C	O5'-P-OP2	-5.15	101.07	105.70
1	2A	333	G	C4-C5-N7	5.15	112.86	110.80
1	2A	619	G	N3-C4-N9	5.15	129.09	126.00
1	2A	855	G	N7-C8-N9	5.15	115.67	113.10
1	2A	1261	C	N3-C2-O2	5.15	125.50	121.90
1	2A	1545	A	C8-N9-C4	-5.15	103.74	105.80
1	2A	2017	U	C4-C5-C6	5.15	122.79	119.70
1	2A	2057	A	OP2-P-O3'	-5.15	93.87	105.20
1	2A	2682	U	OP1-P-OP2	5.15	127.32	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2B	1	U	C2-N1-C1'	5.15	123.88	117.70
1	1A	660	G	C4-C5-N7	5.15	112.86	110.80
1	1A	1025	G	C5-N7-C8	5.15	106.87	104.30
1	1A	2066	C	N1-C2-N3	-5.15	115.60	119.20
32	1a	509	A	C5-C6-N6	5.15	127.82	123.70
32	1a	765	G	C8-N9-C4	5.15	108.46	106.40
1	2A	220	G	C6-C5-N7	-5.15	127.31	130.40
1	2A	2060	A	N9-C4-C5	5.15	107.86	105.80
1	1A	414	C	OP2-P-O3'	5.14	116.52	105.20
1	1A	734	A	C6-N1-C2	5.14	121.69	118.60
1	1A	1343	G	C5-N7-C8	-5.14	101.73	104.30
2	1B	86	G	C5-C6-O6	-5.14	125.51	128.60
32	1a	1084	G	C4-C5-C6	5.14	121.89	118.80
1	2A	15	G	C8-N9-C4	5.14	108.46	106.40
1	2A	2261	C	C5-C6-N1	-5.14	118.43	121.00
32	2a	326	G	C5-C6-O6	5.14	131.69	128.60
1	1A	215	G	C4-C5-C6	5.14	121.89	118.80
1	1A	559	G	C2-N3-C4	-5.14	109.33	111.90
1	1A	793	A	OP1-P-O3'	5.14	116.52	105.20
1	1A	2688	U	OP1-P-OP2	-5.14	111.89	119.60
32	1a	1027	C	C2-N3-C4	5.14	122.47	119.90
1	2A	815	C	O5'-P-OP2	-5.14	101.07	105.70
1	2A	2494	G	C2-N3-C4	-5.14	109.33	111.90
2	2B	50	G	C8-N9-C4	-5.14	104.34	106.40
32	2a	531	U	N1-C2-N3	-5.14	111.81	114.90
1	1A	180	G	N1-C2-N2	5.14	120.83	116.20
1	1A	1213	A	C4-C5-C6	5.14	119.57	117.00
1	1A	1621	U	OP2-P-O3'	-5.14	93.89	105.20
1	1A	1759	A	OP1-P-OP2	5.14	127.31	119.60
1	1A	2319	G	N3-C4-N9	5.14	129.08	126.00
1	1A	2379	G	C5-C6-O6	-5.14	125.52	128.60
1	2A	377	C	C2-N1-C1'	-5.14	113.14	118.80
1	2A	1616	A	C5-N7-C8	-5.14	101.33	103.90
32	2a	803	G	C2-N3-C4	-5.14	109.33	111.90
1	1A	189	G	C6-N1-C2	-5.14	122.02	125.10
1	1A	203	C	N3-C4-C5	5.14	123.95	121.90
1	1A	1392	A	C4-C5-N7	-5.14	108.13	110.70
1	1A	1642	G	N3-C4-N9	-5.14	122.92	126.00
1	1A	1816	G	N3-C4-N9	-5.14	122.92	126.00
32	1a	833	U	C4-C5-C6	5.14	122.78	119.70
1	2A	944	G	C8-N9-C4	-5.14	104.34	106.40
1	2A	1638	C	C2-N1-C1'	-5.14	113.15	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2517	C	N3-C4-C5	5.14	123.95	121.90
32	2a	552	U	C2-N3-C4	-5.14	123.92	127.00
1	1A	201	C	C6-N1-C1'	-5.14	114.64	120.80
1	1A	597	U	C5-C6-N1	-5.14	120.13	122.70
32	1a	172	A	N9-C4-C5	5.14	107.86	105.80
32	1a	1442	G	O4'-C1'-N9	-5.14	104.09	108.20
32	2a	993	G	C4-N9-C1'	5.14	133.18	126.50
1	1A	363(B)	G	N3-C4-N9	5.14	129.08	126.00
1	1A	921	G	N7-C8-N9	5.14	115.67	113.10
1	1A	1674	G	N7-C8-N9	-5.14	110.53	113.10
1	1A	1698	A	N1-C2-N3	5.14	131.87	129.30
1	1A	2627	G	C5-N7-C8	-5.14	101.73	104.30
25	13	31	LEU	CA-CB-CG	5.14	127.12	115.30
27	15	15	ARG	NE-CZ-NH1	-5.14	117.73	120.30
32	1a	1481	U	OP2-P-O3'	5.14	116.50	105.20
50	1s	5	LEU	CA-CB-CG	5.14	127.11	115.30
1	2A	189	G	C4-C5-N7	-5.14	108.75	110.80
1	2A	203	C	N3-C2-O2	5.14	125.50	121.90
1	2A	960	A	N9-C4-C5	-5.14	103.75	105.80
1	2A	1352	U	C5-C4-O4	5.14	128.98	125.90
1	2A	1380	G	C2-N3-C4	-5.14	109.33	111.90
1	2A	1614	A	N1-C2-N3	5.14	131.87	129.30
1	2A	2147	G	N1-C2-N3	5.14	126.98	123.90
1	2A	2699	C	C4-C5-C6	5.14	119.97	117.40
1	1A	363(C)	G	C2-N3-C4	5.13	114.47	111.90
1	1A	1041	C	N3-C4-C5	-5.13	119.85	121.90
1	1A	1129	A	OP1-P-O3'	5.13	116.49	105.20
1	1A	1175	U	P-O3'-C3'	5.13	125.86	119.70
1	1A	1783	A	N9-C4-C5	5.13	107.85	105.80
1	1A	2061	G	N1-C6-O6	-5.13	116.82	119.90
1	1A	2476	A	O4'-C1'-N9	-5.13	104.09	108.20
1	1A	2514	U	C5-C4-O4	-5.13	122.82	125.90
32	1a	541	G	N9-C1'-C2'	-5.13	106.35	112.00
32	1a	561	U	OP1-P-O3'	5.13	116.50	105.20
1	2A	2021	C	N3-C2-O2	-5.13	118.31	121.90
32	2a	485	G	C2-N3-C4	5.13	114.47	111.90
1	1A	501	A	OP1-P-O3'	5.13	116.49	105.20
1	1A	2019	A	P-O3'-C3'	5.13	125.86	119.70
1	1A	2682	U	C2-N3-C4	-5.13	123.92	127.00
1	2A	420	C	N3-C4-N4	-5.13	114.41	118.00
1	1A	172	C	C6-N1-C2	-5.13	118.25	120.30
1	1A	339	U	C5-C4-O4	5.13	128.98	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	478	A	C4-C5-C6	5.13	119.57	117.00
1	1A	681	G	C5-C6-O6	-5.13	125.52	128.60
1	1A	776	G	N3-C4-C5	-5.13	126.03	128.60
1	1A	961	C	O5'-P-OP2	-5.13	101.08	105.70
1	1A	1020	A	C5-C6-N6	5.13	127.80	123.70
1	1A	2313	C	OP2-P-O3'	5.13	116.49	105.20
1	1A	2858	C	N3-C4-C5	5.13	123.95	121.90
32	1a	362	G	N9-C4-C5	5.13	107.45	105.40
32	1a	902	G	C5-C6-O6	-5.13	125.52	128.60
1	2A	229	A	N7-C8-N9	5.13	116.37	113.80
1	2A	769	G	C2-N3-C4	-5.13	109.33	111.90
1	2A	980	A	C4-C5-N7	5.13	113.27	110.70
1	2A	1420	U	P-O3'-C3'	5.13	125.86	119.70
1	2A	2677	G	N7-C8-N9	5.13	115.67	113.10
1	2A	2807	G	C5-C6-O6	5.13	131.68	128.60
1	1A	684	G	C2-N3-C4	5.13	114.47	111.90
1	1A	1814	G	C4-C5-N7	-5.13	108.75	110.80
1	1A	2680	C	C4-C5-C6	-5.13	114.83	117.40
1	1A	2731	G	C4-C5-N7	5.13	112.85	110.80
1	2A	1568	G	O4'-C1'-N9	-5.13	104.10	108.20
1	2A	2340	G	C8-N9-C4	5.13	108.45	106.40
1	1A	429	A	O5'-P-OP1	-5.13	101.08	105.70
1	1A	465	G	N3-C2-N2	5.13	123.49	119.90
1	1A	729	G	C5-N7-C8	-5.13	101.74	104.30
1	1A	947	G	N7-C8-N9	5.13	115.67	113.10
1	1A	1150	C	OP1-P-OP2	-5.13	111.91	119.60
1	1A	1706	U	C6-N1-C2	5.13	124.08	121.00
32	1a	33	A	C8-N9-C4	5.13	107.85	105.80
32	1a	1287	A	C6-N1-C2	5.13	121.68	118.60
1	2A	95	G	N3-C2-N2	-5.13	116.31	119.90
1	2A	1284	A	C5-C6-N6	-5.13	119.60	123.70
2	2B	80	U	C5-C4-O4	5.13	128.98	125.90
32	2a	1159	U	C6-N1-C2	-5.13	117.92	121.00
1	1A	397	G	C2-N3-C4	-5.13	109.34	111.90
1	1A	738	G	OP1-P-O3'	-5.13	93.92	105.20
1	1A	789	A	C6-C5-N7	-5.13	128.71	132.30
1	1A	1406	U	N3-C2-O2	-5.13	118.61	122.20
1	1A	1787	A	C4-C5-N7	5.13	113.26	110.70
1	1A	2846	G	C5-C6-N1	-5.13	108.94	111.50
1	2A	517	C	C5-C4-N4	-5.13	116.61	120.20
1	2A	563	G	C4-C5-N7	5.13	112.85	110.80
1	2A	2731	G	N3-C4-N9	5.13	129.08	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	233	C	C6-N1-C2	-5.12	118.25	120.30
32	1a	1016	A	C8-N9-C4	5.12	107.85	105.80
1	2A	462	C	C4-C5-C6	5.12	119.96	117.40
1	2A	2092	U	N3-C4-O4	5.12	122.99	119.40
1	1A	1606	G	C6-C5-N7	-5.12	127.33	130.40
1	1A	1649	G	N1-C6-O6	-5.12	116.83	119.90
1	1A	1667	G	C5-C6-O6	-5.12	125.53	128.60
32	1a	14	U	O5'-P-OP2	5.12	116.85	110.70
32	1a	491	G	N3-C4-N9	-5.12	122.93	126.00
1	2A	1137	G	N1-C6-O6	5.12	122.97	119.90
1	2A	1823	G	O5'-P-OP1	-5.12	101.09	105.70
2	2B	55	U	C6-N1-C2	-5.12	117.93	121.00
1	1A	231	C	N1-C2-N3	5.12	122.78	119.20
1	1A	245	G	N1-C2-N3	-5.12	120.83	123.90
1	1A	785	G	C2-N3-C4	5.12	114.46	111.90
1	1A	1551	C	C5-C6-N1	5.12	123.56	121.00
1	1A	1695	G	C8-N9-C1'	-5.12	120.34	127.00
1	1A	2550	G	OP1-P-O3'	5.12	116.47	105.20
1	1A	2859	G	C8-N9-C1'	-5.12	120.34	127.00
1	2A	1108	U	C5-C4-O4	-5.12	122.83	125.90
1	2A	1501	C	N3-C2-O2	5.12	125.48	121.90
1	2A	1635	G	C5-C6-O6	-5.12	125.53	128.60
1	2A	2134	A	C2-N3-C4	5.12	113.16	110.60
32	2a	1294	G	C8-N9-C1'	5.12	133.66	127.00
32	2a	1437	C	C6-N1-C2	5.12	122.35	120.30
1	1A	1764	G	N9-C4-C5	5.12	107.45	105.40
1	1A	2838	G	C5-N7-C8	-5.12	101.74	104.30
32	1a	66	G	N7-C8-N9	5.12	115.66	113.10
1	2A	2729	G	N1-C6-O6	5.12	122.97	119.90
32	2a	781	A	N9-C4-C5	5.12	107.85	105.80
1	1A	532	A	C2-N3-C4	5.12	113.16	110.60
1	1A	765	G	C6-C5-N7	-5.12	127.33	130.40
1	1A	961	C	N3-C2-O2	-5.12	118.32	121.90
1	1A	970	C	O5'-P-OP2	-5.12	101.09	105.70
1	1A	1219	G	C5-C6-O6	-5.12	125.53	128.60
1	1A	1773	A	N9-C1'-C2'	-5.12	106.37	112.00
1	1A	1778	U	C6-N1-C2	5.12	124.07	121.00
1	1A	2850	A	C8-N9-C4	5.12	107.85	105.80
1	2A	760	G	C2-N3-C4	-5.12	109.34	111.90
1	2A	1309	G	C2-N3-C4	-5.12	109.34	111.90
1	2A	2323	G	OP1-P-OP2	5.12	127.28	119.60
1	1A	1259	G	OP1-P-OP2	-5.12	111.92	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2371	G	N3-C4-N9	5.12	129.07	126.00
1	2A	932	G	N1-C6-O6	-5.12	116.83	119.90
32	2a	524	G	N7-C8-N9	5.12	115.66	113.10
1	1A	44	G	OP2-P-O3'	5.12	116.46	105.20
1	1A	379	G	N1-C6-O6	-5.12	116.83	119.90
1	1A	596	G	N9-C4-C5	-5.12	103.35	105.40
2	1B	79	C	N1-C2-O2	5.12	121.97	118.90
32	1a	687	A	P-O3'-C3'	5.12	125.84	119.70
1	2A	938	G	C2-N3-C4	-5.12	109.34	111.90
1	2A	1587	A	C2-N3-C4	5.12	113.16	110.60
32	2a	471	G	N3-C4-N9	5.12	129.07	126.00
1	1A	13	A	N9-C4-C5	5.11	107.85	105.80
1	1A	1289	C	OP2-P-O3'	5.11	116.45	105.20
1	2A	751	A	N3-C4-C5	-5.11	123.22	126.80
1	2A	1308	A	N1-C2-N3	5.11	131.86	129.30
1	2A	1781	C	C6-N1-C1'	5.11	126.94	120.80
32	2a	47	C	C6-N1-C2	-5.11	118.25	120.30
1	1A	1052	C	N1-C2-O2	5.11	121.97	118.90
1	1A	2363	C	O5'-P-OP2	-5.11	101.10	105.70
32	1a	1424	C	C5-C6-N1	-5.11	118.44	121.00
1	2A	135	G	N9-C1'-C2'	-5.11	106.38	112.00
1	2A	322	A	C5-C6-N6	-5.11	119.61	123.70
1	2A	990	A	OP1-P-OP2	-5.11	111.93	119.60
1	2A	2182	G	C5-C6-O6	5.11	131.67	128.60
32	2a	1527	C	C6-N1-C2	5.11	122.34	120.30
1	1A	271(B)	C	N3-C4-C5	5.11	123.94	121.90
1	1A	1137	G	C5-C6-O6	-5.11	125.53	128.60
1	1A	1767	C	C6-N1-C2	5.11	122.34	120.30
1	1A	2378	A	N9-C4-C5	-5.11	103.76	105.80
1	1A	2461	C	C6-N1-C2	-5.11	118.26	120.30
1	1A	2706	G	OP1-P-OP2	5.11	127.26	119.60
1	2A	979	G	C5-C6-O6	5.11	131.67	128.60
1	2A	1252	G	O4'-C1'-N9	-5.11	104.11	108.20
1	2A	1778	U	N3-C2-O2	-5.11	118.62	122.20
1	1A	2254	C	N1-C2-O2	-5.11	115.83	118.90
2	1B	45	A	OP1-P-O3'	5.11	116.44	105.20
1	2A	95	G	C5-N7-C8	-5.11	101.75	104.30
1	2A	1200	C	C2-N3-C4	-5.11	117.35	119.90
1	2A	2384	G	O5'-P-OP2	-5.11	101.10	105.70
32	2a	471	G	C6-C5-N7	-5.11	127.33	130.40
1	1A	338	G	C6-N1-C2	-5.11	122.03	125.10
1	1A	428	A	C2-N3-C4	-5.11	108.05	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	528	A	C6-N1-C2	-5.11	115.53	118.60
1	1A	573	G	P-O3'-C3'	-5.11	113.57	119.70
1	1A	964	C	C6-N1-C1'	-5.11	114.67	120.80
1	1A	1541	G	N3-C4-C5	-5.11	126.05	128.60
1	1A	2206	G	O4'-C1'-N9	5.11	112.28	108.20
1	1A	2445	G	C2-N3-C4	5.11	114.45	111.90
1	1A	2461	C	O5'-P-OP2	-5.11	101.10	105.70
1	1A	2600	A	N1-C6-N6	-5.11	115.54	118.60
2	1B	6	C	C6-N1-C2	5.11	122.34	120.30
1	2A	737	C	C5-C6-N1	-5.11	118.45	121.00
1	2A	800	A	OP2-P-O3'	5.11	116.44	105.20
1	2A	1065	U	N3-C4-O4	-5.11	115.83	119.40
1	2A	1271	G	O5'-P-OP2	-5.11	101.10	105.70
33	2b	23	ARG	N-CA-C	-5.11	97.21	111.00
1	1A	198	C	N3-C4-C5	-5.11	119.86	121.90
1	1A	332	A	N1-C2-N3	5.11	131.85	129.30
1	1A	530	G	C8-N9-C4	5.11	108.44	106.40
1	1A	557	U	OP1-P-OP2	5.11	127.26	119.60
1	1A	568	U	C4-C5-C6	-5.11	116.64	119.70
1	1A	573	G	C5-N7-C8	-5.11	101.75	104.30
1	1A	1092	C	C2-N3-C4	5.11	122.45	119.90
1	1A	1779	U	C2-N3-C4	5.11	130.06	127.00
1	1A	2274	A	OP1-P-OP2	-5.11	111.94	119.60
1	1A	2406	U	C5-C6-N1	5.11	125.25	122.70
1	1A	2740	A	C6-N1-C2	-5.11	115.54	118.60
1	2A	248	G	C8-N9-C1'	5.11	133.64	127.00
1	2A	1589	C	O5'-P-OP1	-5.11	101.11	105.70
1	2A	2005	A	OP1-P-O3'	5.11	116.43	105.20
32	2a	543	C	C6-N1-C2	-5.11	118.26	120.30
32	2a	981	U	C5-C6-N1	5.11	125.25	122.70
32	1a	829	G	N1-C6-O6	5.10	122.96	119.90
1	2A	614	U	O5'-P-OP2	5.10	116.83	110.70
1	2A	760	G	N3-C2-N2	-5.10	116.33	119.90
1	1A	715	G	C6-C5-N7	-5.10	127.34	130.40
1	1A	863	A	OP2-P-O3'	5.10	116.43	105.20
1	1A	1237	A	C8-N9-C4	-5.10	103.76	105.80
1	1A	1421	G	C4-C5-N7	5.10	112.84	110.80
1	1A	1554	A	C4-C5-C6	-5.10	114.45	117.00
7	1H	3	ARG	NE-CZ-NH1	-5.10	117.75	120.30
32	1a	872	A	N1-C6-N6	5.10	121.66	118.60
2	2B	113	G	C8-N9-C1'	5.10	133.63	127.00
32	2a	798	G	N1-C6-O6	-5.10	116.84	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2508	G	C2-N3-C4	5.10	114.45	111.90
1	1A	2618	G	C4-C5-N7	-5.10	108.76	110.80
1	2A	1169	G	C8-N9-C4	-5.10	104.36	106.40
1	2A	1224	C	C5-C6-N1	-5.10	118.45	121.00
1	1A	747	U	C2-N1-C1'	5.10	123.82	117.70
1	1A	939	G	N1-C6-O6	-5.10	116.84	119.90
1	1A	1037	G	N3-C4-C5	5.10	131.15	128.60
1	1A	1902	C	C5-C6-N1	5.10	123.55	121.00
1	1A	2726	U	C5-C6-N1	-5.10	120.15	122.70
32	1a	15	G	N3-C4-N9	5.10	129.06	126.00
32	1a	1030	C	C6-N1-C2	-5.10	118.26	120.30
1	2A	1389	G	N1-C6-O6	5.10	122.96	119.90
1	2A	1655	A	C8-N9-C4	5.10	107.84	105.80
32	2a	781	A	C5-C6-N6	5.10	127.78	123.70
32	2a	1054	C	C6-N1-C1'	-5.10	114.68	120.80
32	2a	1435	G	N1-C2-N3	5.10	126.96	123.90
1	1A	119	A	N1-C2-N3	5.10	131.85	129.30
1	1A	615	G	N1-C2-N2	-5.10	111.61	116.20
1	1A	932	G	N9-C4-C5	5.10	107.44	105.40
1	1A	1435	G	C4-C5-N7	5.10	112.84	110.80
1	1A	2053	G	N9-C1'-C2'	-5.10	106.39	112.00
1	1A	2235	G	C5-C6-O6	5.10	131.66	128.60
32	1a	1276	G	N7-C8-N9	5.10	115.65	113.10
1	2A	1584	C	C4-C5-C6	5.10	119.95	117.40
1	2A	2009	G	C8-N9-C4	5.10	108.44	106.40
1	2A	2016	U	N3-C4-C5	-5.10	111.54	114.60
1	2A	2250	G	C2-N3-C4	5.10	114.45	111.90
1	2A	2688	U	OP1-P-O3'	5.10	116.42	105.20
27	25	58	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	1A	1758	G	C5-N7-C8	-5.10	101.75	104.30
1	1A	2073	C	OP2-P-O3'	5.10	116.41	105.20
1	1A	2622	C	C6-N1-C2	5.10	122.34	120.30
1	2A	2137	C	C5-C6-N1	5.10	123.55	121.00
1	2A	2137	C	C6-N1-C2	-5.10	118.26	120.30
1	2A	2468	G	N3-C4-C5	5.10	131.15	128.60
1	2A	2718	G	N1-C6-O6	5.10	122.96	119.90
1	1A	495	G	N3-C2-N2	-5.09	116.33	119.90
1	1A	762	U	O5'-P-OP1	-5.09	101.11	105.70
1	1A	785	G	C8-N9-C4	-5.09	104.36	106.40
1	1A	1403	C	O5'-P-OP1	-5.09	101.11	105.70
1	1A	1986	A	N7-C8-N9	-5.09	111.25	113.80
1	1A	2334	G	N3-C2-N2	5.09	123.47	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2564	A	C6-C5-N7	-5.09	128.74	132.30
32	1a	286	G	C5-C6-O6	5.09	131.66	128.60
1	2A	489	G	C4-N9-C1'	5.09	133.12	126.50
1	2A	2087	G	N1-C6-O6	5.09	122.96	119.90
1	2A	2271	G	OP2-P-O3'	5.09	116.41	105.20
32	2a	1261	A	C6-C5-N7	-5.09	128.73	132.30
32	2a	1509	C	C2-N3-C4	-5.09	117.35	119.90
1	1A	16	G	N3-C4-N9	-5.09	122.94	126.00
1	1A	1274	A	C5-C6-N6	-5.09	119.62	123.70
1	1A	1972	A	OP2-P-O3'	5.09	116.40	105.20
1	2A	870	A	C8-N9-C4	5.09	107.84	105.80
1	2A	914	C	C5-C4-N4	5.09	123.77	120.20
1	2A	2848	G	O4'-C1'-N9	5.09	112.27	108.20
1	1A	1051	G	O5'-P-OP2	5.09	116.81	110.70
1	1A	2051	A	N7-C8-N9	-5.09	111.25	113.80
1	1A	2078	C	O5'-P-OP1	-5.09	101.12	105.70
32	1a	482	A	OP1-P-O3'	5.09	116.40	105.20
32	1a	585	G	C8-N9-C1'	-5.09	120.38	127.00
1	2A	2187	G	N1-C6-O6	5.09	122.95	119.90
1	2A	2562	U	O5'-P-OP1	5.09	116.81	110.70
1	2A	2787	C	N3-C2-O2	-5.09	118.33	121.90
1	1A	620	G	N3-C4-N9	5.09	129.05	126.00
1	1A	776	G	C4-C5-C6	5.09	121.85	118.80
1	1A	1174	A	P-O3'-C3'	5.09	125.81	119.70
1	1A	1703	G	N3-C2-N2	-5.09	116.34	119.90
1	1A	2074	U	C2-N1-C1'	5.09	123.81	117.70
20	1Y	10	GLY	N-CA-C	-5.09	100.38	113.10
32	1a	337	C	N1-C2-O2	5.09	121.95	118.90
1	2A	614(C)	A	C4-C5-C6	5.09	119.55	117.00
1	2A	1109	C	C5-C6-N1	5.09	123.55	121.00
32	2a	1506	U	N1-C2-O2	5.09	126.36	122.80
1	1A	251	A	N3-C4-N9	5.09	131.47	127.40
1	1A	380	U	C5-C4-O4	-5.09	122.85	125.90
1	1A	2280	G	C5-C6-O6	5.09	131.65	128.60
1	2A	738	G	P-O3'-C3'	-5.09	113.59	119.70
1	1A	329	G	N1-C2-N3	-5.09	120.85	123.90
1	1A	1000	A	C6-N1-C2	5.09	121.65	118.60
1	1A	1325	G	C8-N9-C4	-5.09	104.37	106.40
1	1A	1338	G	OP2-P-O3'	-5.09	94.01	105.20
1	1A	2179	C	C6-N1-C2	-5.09	118.27	120.30
1	1A	2572	A	N1-C6-N6	5.09	121.65	118.60
1	1A	2733	A	C5-C6-N6	-5.09	119.63	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2827	C	N3-C4-C5	5.09	123.94	121.90
32	1a	73	G	C4-C5-N7	-5.09	108.77	110.80
1	2A	197	A	C4-C5-N7	5.09	113.24	110.70
1	2A	983	A	OP2-P-O3'	5.09	116.39	105.20
1	2A	1234	U	C5-C4-O4	5.09	128.95	125.90
2	2B	108	U	O5'-P-OP2	-5.09	101.12	105.70
32	2a	128	G	N1-C6-O6	5.09	122.95	119.90
32	2a	770	C	N3-C4-C5	-5.09	119.86	121.90
1	1A	534	U	C6-N1-C2	5.08	124.05	121.00
1	1A	1564	C	N3-C2-O2	-5.08	118.34	121.90
1	1A	2623	G	C5-C6-O6	-5.08	125.55	128.60
32	1a	129	U	O5'-P-OP2	-5.08	101.12	105.70
32	2a	375	U	O5'-P-OP1	-5.08	101.12	105.70
32	2a	1246	C	C6-N1-C2	-5.08	118.27	120.30
1	1A	76	C	N3-C4-N4	5.08	121.56	118.00
1	1A	985	C	N3-C2-O2	-5.08	118.34	121.90
1	1A	1427	A	N9-C4-C5	5.08	107.83	105.80
1	1A	1428	C	N3-C4-N4	-5.08	114.44	118.00
1	1A	1436	G	N3-C4-C5	5.08	131.14	128.60
1	1A	1527	G	N1-C2-N3	5.08	126.95	123.90
1	1A	2513	G	C5-N7-C8	-5.08	101.76	104.30
1	1A	2660	A	OP1-P-O3'	5.08	116.38	105.20
1	2A	1093	G	N3-C4-C5	-5.08	126.06	128.60
1	2A	1382	G	C8-N9-C4	5.08	108.43	106.40
1	2A	2756	U	OP1-P-O3'	5.08	116.38	105.20
32	2a	22	G	C5-C6-O6	-5.08	125.55	128.60
32	2a	41	G	N1-C2-N2	5.08	120.77	116.20
32	2a	1522	U	N1-C2-N3	5.08	117.95	114.90
1	1A	919	G	C8-N9-C4	-5.08	104.37	106.40
1	1A	944	G	C4-N9-C1'	5.08	133.11	126.50
1	1A	1711	C	OP2-P-O3'	5.08	116.38	105.20
1	1A	2440	C	C5-C6-N1	-5.08	118.46	121.00
1	1A	2825	C	N1-C2-O2	-5.08	115.85	118.90
22	10	82	ARG	NE-CZ-NH1	5.08	122.84	120.30
32	1a	268	C	C6-N1-C2	-5.08	118.27	120.30
32	1a	1122	U	C6-N1-C2	-5.08	117.95	121.00
1	2A	381	G	C5-C6-O6	5.08	131.65	128.60
1	2A	564	C	C4-C5-C6	5.08	119.94	117.40
1	2A	978	G	O5'-P-OP1	-5.08	101.13	105.70
1	2A	2179	C	C2-N3-C4	5.08	122.44	119.90
32	2a	168	G	N3-C4-C5	-5.08	126.06	128.60
1	1A	528	A	C5-N7-C8	-5.08	101.36	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1359	A	C2-N3-C4	5.08	113.14	110.60
1	1A	2767	C	N3-C2-O2	-5.08	118.34	121.90
32	1a	572	A	C6-C5-N7	5.08	135.86	132.30
32	1a	595	G	C4-N9-C1'	5.08	133.10	126.50
1	2A	642	G	C4-C5-N7	-5.08	108.77	110.80
1	2A	1660	C	C5-C4-N4	5.08	123.76	120.20
1	1A	104	U	N3-C2-O2	5.08	125.76	122.20
1	1A	2197	U	OP2-P-O3'	5.08	116.37	105.20
1	1A	2498	C	OP1-P-OP2	-5.08	111.98	119.60
1	1A	2758	A	C8-N9-C4	5.08	107.83	105.80
1	2A	668	G	C2-N3-C4	-5.08	109.36	111.90
1	2A	800	A	C5-C6-N6	5.08	127.76	123.70
1	2A	864	G	N3-C4-C5	-5.08	126.06	128.60
1	2A	1147	C	C4-C5-C6	5.08	119.94	117.40
1	2A	1953	A	C4-C5-C6	5.08	119.54	117.00
1	2A	2022	U	O5'-P-OP1	-5.08	101.13	105.70
1	2A	2556	C	N3-C4-N4	5.08	121.56	118.00
32	2a	975	A	C5-N7-C8	-5.08	101.36	103.90
32	2a	1203	C	C6-N1-C2	5.08	122.33	120.30
1	1A	2627	G	C6-N1-C2	-5.08	122.05	125.10
32	1a	871	U	OP2-P-O3'	5.08	116.37	105.20
32	1a	1529	G	C5-N7-C8	-5.08	101.76	104.30
1	2A	252	G	C5-N7-C8	5.08	106.84	104.30
1	1A	100	G	C8-N9-C4	5.08	108.43	106.40
1	1A	205	G	OP1-P-OP2	5.08	127.21	119.60
1	1A	934	G	N9-C4-C5	-5.08	103.37	105.40
1	1A	984	A	N1-C6-N6	5.08	121.64	118.60
1	1A	1220	A	O4'-C1'-N9	5.08	112.26	108.20
1	1A	1310	G	C5-C6-O6	-5.08	125.56	128.60
1	1A	1938	A	N9-C4-C5	5.08	107.83	105.80
1	1A	2377	A	C2-N3-C4	-5.08	108.06	110.60
32	1a	807	A	N9-C4-C5	5.08	107.83	105.80
32	1a	873	A	C2-N3-C4	5.08	113.14	110.60
1	2A	210	C	O5'-P-OP1	5.08	116.79	110.70
1	2A	718	A	C4-N9-C1'	5.08	135.44	126.30
1	1A	27	G	C5'-C4'-O4'	-5.07	103.01	109.10
1	1A	45	C	OP1-P-O3'	-5.07	94.04	105.20
1	1A	186	G	C8-N9-C4	5.07	108.43	106.40
1	1A	432	A	C6-C5-N7	-5.07	128.75	132.30
1	1A	768	G	C5-N7-C8	-5.07	101.76	104.30
1	1A	1282	U	C2-N1-C1'	-5.07	111.61	117.70
2	1B	1	U	C2-N1-C1'	5.07	123.79	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1B	89	G	C8-N9-C4	5.07	108.43	106.40
1	2A	480	A	N7-C8-N9	5.07	116.34	113.80
1	2A	738	G	O5'-P-OP2	-5.07	101.13	105.70
1	2A	1643	G	N1-C6-O6	5.07	122.94	119.90
1	2A	2017	U	C5-C4-O4	5.07	128.94	125.90
1	2A	2488	A	C5-C6-N1	-5.07	115.16	117.70
2	2B	22	U	C6-N1-C2	-5.07	117.96	121.00
2	2B	37	C	OP2-P-O3'	5.07	116.36	105.20
32	2a	273	A	C2-N3-C4	-5.07	108.06	110.60
44	2m	116	THR	N-CA-C	5.07	124.70	111.00
1	1A	258	G	C5-N7-C8	-5.07	101.76	104.30
1	1A	258	G	N7-C8-N9	5.07	115.64	113.10
1	1A	529	A	O4'-C1'-N9	5.07	112.26	108.20
1	1A	2142	C	C6-N1-C2	-5.07	118.27	120.30
1	1A	2693	A	C5-C6-N6	-5.07	119.64	123.70
1	1A	662	G	C8-N9-C4	-5.07	104.37	106.40
1	1A	682	G	C8-N9-C4	5.07	108.43	106.40
1	1A	776	G	C2-N3-C4	-5.07	109.36	111.90
1	1A	1162	G	C8-N9-C1'	5.07	133.59	127.00
1	1A	1406	U	C2-N3-C4	-5.07	123.96	127.00
1	2A	183	C	C6-N1-C2	5.07	122.33	120.30
1	2A	188	G	C6-C5-N7	-5.07	127.36	130.40
1	2A	620	G	O5'-P-OP2	-5.07	101.14	105.70
1	2A	809	G	C5-C6-N1	5.07	114.03	111.50
1	2A	1333	C	OP1-P-OP2	-5.07	112.00	119.60
1	2A	1410	G	C5-C6-O6	5.07	131.64	128.60
1	2A	1800	C	N1-C2-N3	5.07	122.75	119.20
32	2a	230	G	N7-C8-N9	5.07	115.64	113.10
36	2e	151	LEU	CA-CB-CG	-5.07	103.64	115.30
1	1A	118	A	C4-C5-C6	-5.07	114.47	117.00
1	1A	861	A	C8-N9-C4	5.07	107.83	105.80
1	1A	2647	U	N1-C2-N3	5.07	117.94	114.90
32	2a	603	U	N3-C2-O2	5.07	125.75	122.20
1	1A	258	G	C4-C5-N7	5.07	112.83	110.80
1	1A	640	C	N3-C2-O2	5.07	125.45	121.90
1	1A	973	A	N1-C6-N6	5.07	121.64	118.60
1	1A	1818	U	C2-N3-C4	-5.07	123.96	127.00
1	1A	1849	G	N9-C4-C5	5.07	107.43	105.40
1	1A	2031	A	O5'-P-OP1	5.07	116.78	110.70
2	1B	1	U	N1-C2-O2	5.07	126.35	122.80
32	1a	244	U	C6-N1-C1'	-5.07	114.11	121.20
32	1a	360	A	C8-N9-C4	-5.07	103.77	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1268	A	N1-C6-N6	-5.07	115.56	118.60
1	2A	631	A	O5'-P-OP2	-5.07	101.14	105.70
1	2A	2875	C	N3-C4-C5	-5.07	119.87	121.90
1	1A	1290	C	C5-C4-N4	5.07	123.75	120.20
1	1A	2664	G	C5-C6-O6	5.07	131.64	128.60
32	1a	220	G	C4-N9-C1'	5.07	133.09	126.50
1	2A	383	U	C6-N1-C2	-5.07	117.96	121.00
1	2A	574	C	N3-C2-O2	5.07	125.45	121.90
1	2A	2218	U	OP2-P-O3'	5.07	116.34	105.20
1	2A	2334	G	O4'-C1'-N9	-5.07	104.15	108.20
1	2A	2346	A	N1-C6-N6	-5.07	115.56	118.60
1	1A	2003	G	C8-N9-C4	5.06	108.43	106.40
1	2A	371	A	N9-C4-C5	-5.06	103.77	105.80
1	2A	1847	A	C8-N9-C4	-5.06	103.77	105.80
1	1A	603	A	N1-C6-N6	-5.06	115.56	118.60
1	1A	1032	A	N7-C8-N9	-5.06	111.27	113.80
1	1A	1328	G	O5'-P-OP1	-5.06	101.14	105.70
1	1A	1645	G	OP2-P-O3'	5.06	116.34	105.20
1	1A	1845	G	N9-C4-C5	5.06	107.42	105.40
32	1a	132	C	C6-N1-C2	5.06	122.33	120.30
32	1a	898	G	N3-C2-N2	-5.06	116.36	119.90
1	2A	10	G	N3-C4-C5	5.06	131.13	128.60
1	2A	84	A	N7-C8-N9	-5.06	111.27	113.80
1	2A	122	G	C5-C6-N1	-5.06	108.97	111.50
1	2A	154	G	C8-N9-C4	5.06	108.42	106.40
1	2A	645	C	C6-N1-C1'	-5.06	114.72	120.80
1	2A	775	G	OP1-P-O3'	5.06	116.34	105.20
1	2A	1806	C	C2-N1-C1'	-5.06	113.23	118.80
1	2A	2182	G	C8-N9-C1'	5.06	133.58	127.00
1	2A	2770	G	C2-N3-C4	5.06	114.43	111.90
32	2a	901	A	N9-C4-C5	-5.06	103.78	105.80
1	1A	145	G	N1-C2-N3	5.06	126.94	123.90
1	1A	992	C	OP1-P-OP2	-5.06	112.01	119.60
1	1A	1165	U	N1-C2-N3	5.06	117.94	114.90
2	1B	116	G	C8-N9-C1'	-5.06	120.42	127.00
32	1a	777	A	O5'-P-OP1	5.06	116.77	110.70
1	2A	726	G	C5-C6-O6	5.06	131.64	128.60
1	2A	798	G	C5-C6-O6	5.06	131.64	128.60
1	2A	1151	G	C8-N9-C1'	5.06	133.58	127.00
1	1A	64	A	C5-C6-N1	5.06	120.23	117.70
1	1A	748	G	C6-N1-C2	-5.06	122.06	125.10
1	1A	867	C	N3-C4-N4	5.06	121.54	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	979	G	N1-C2-N2	5.06	120.75	116.20
1	1A	1306	C	N3-C4-C5	5.06	123.92	121.90
1	1A	1769	G	N1-C2-N3	5.06	126.94	123.90
32	1a	772	U	C5-C6-N1	5.06	125.23	122.70
32	1a	1467	G	N9-C4-C5	5.06	107.42	105.40
1	2A	448	U	N3-C4-O4	5.06	122.94	119.40
2	2B	8	U	N3-C2-O2	5.06	125.74	122.20
32	2a	222	U	N3-C2-O2	-5.06	118.66	122.20
32	2a	594	G	C8-N9-C4	-5.06	104.38	106.40
1	1A	141	A	N9-C4-C5	-5.06	103.78	105.80
1	1A	226	G	N1-C2-N2	5.06	120.75	116.20
1	1A	740	U	P-O3'-C3'	-5.06	113.63	119.70
1	1A	818	G	C5-N7-C8	-5.06	101.77	104.30
1	1A	1061	U	N1-C2-O2	5.06	126.34	122.80
1	1A	1351	C	OP1-P-O3'	5.06	116.33	105.20
1	1A	1460	A	O4'-C1'-N9	5.06	112.25	108.20
1	1A	2347	C	N3-C4-C5	5.06	123.92	121.90
1	1A	2609	U	N3-C2-O2	-5.06	118.66	122.20
32	1a	1087	G	C2-N3-C4	5.06	114.43	111.90
32	1a	1510	U	C4-C5-C6	5.06	122.73	119.70
1	2A	1978	A	OP2-P-O3'	5.06	116.33	105.20
1	2A	2297	C	C5-C6-N1	-5.06	118.47	121.00
1	2A	2546	U	C4-C5-C6	5.06	122.73	119.70
1	1A	808	G	OP1-P-O3'	5.06	116.32	105.20
1	1A	949	C	C5-C4-N4	5.06	123.74	120.20
1	1A	987	G	N9-C4-C5	5.06	107.42	105.40
1	1A	1363	C	OP1-P-OP2	5.06	127.18	119.60
1	1A	2275	C	C4-C5-C6	5.06	119.93	117.40
1	1A	2547	U	N1-C2-O2	-5.06	119.26	122.80
1	1A	48	G	C5-C6-O6	5.05	131.63	128.60
1	1A	73	A	C5-C6-N1	5.05	120.23	117.70
1	1A	109	G	C5-C6-O6	5.05	131.63	128.60
1	1A	121	G	C8-N9-C4	-5.05	104.38	106.40
1	1A	1242	A	C6-N1-C2	-5.05	115.57	118.60
1	1A	2623	G	N3-C4-C5	-5.05	126.07	128.60
2	1B	73	A	C8-N9-C4	-5.05	103.78	105.80
32	1a	331	G	N1-C6-O6	5.05	122.93	119.90
1	2A	1317	A	N7-C8-N9	-5.05	111.27	113.80
1	2A	1793	C	C2-N1-C1'	-5.05	113.24	118.80
1	2A	2407	G	C4-N9-C1'	5.05	133.07	126.50
1	2A	2639	A	C2-N3-C4	-5.05	108.07	110.60
1	2A	2720	U	C4-C5-C6	5.05	122.73	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1366	C	C6-N1-C2	-5.05	118.28	120.30
32	2a	1416	G	C5-C6-N1	-5.05	108.97	111.50
1	1A	670	A	C6-C5-N7	-5.05	128.76	132.30
1	1A	1162	G	C4-N9-C1'	-5.05	119.93	126.50
1	1A	1769	G	N1-C6-O6	5.05	122.93	119.90
1	2A	2433	A	O5'-P-OP1	5.05	116.76	110.70
2	2B	103	G	O5'-P-OP2	-5.05	101.15	105.70
1	1A	137	C	N3-C4-C5	-5.05	119.88	121.90
1	1A	2855	C	C5-C6-N1	5.05	123.53	121.00
2	1B	99	G	C2-N3-C4	-5.05	109.37	111.90
32	1a	441	A	C8-N9-C4	-5.05	103.78	105.80
1	2A	816	C	C5-C4-N4	-5.05	116.66	120.20
1	2A	979	G	C5-N7-C8	5.05	106.83	104.30
1	2A	2571	C	O5'-P-OP2	-5.05	101.15	105.70
1	1A	51	G	C5-N7-C8	5.05	106.82	104.30
1	1A	371	A	C5-C6-N6	-5.05	119.66	123.70
1	1A	460	A	N1-C6-N6	-5.05	115.57	118.60
1	1A	643	A	C8-N9-C4	5.05	107.82	105.80
1	1A	836	G	C8-N9-C4	-5.05	104.38	106.40
1	1A	1164	G	N7-C8-N9	-5.05	110.58	113.10
1	1A	2089	U	N3-C4-C5	5.05	117.63	114.60
32	1a	1431	C	N3-C2-O2	5.05	125.44	121.90
1	2A	543	C	C6-N1-C2	5.05	122.32	120.30
1	2A	593	G	C6-C5-N7	-5.05	127.37	130.40
1	2A	734	A	C8-N9-C4	5.05	107.82	105.80
1	2A	800	A	N3-C4-N9	-5.05	123.36	127.40
1	2A	859	G	O4'-C1'-N9	-5.05	104.16	108.20
1	2A	1976	U	N1-C2-N3	5.05	117.93	114.90
1	2A	2178	C	C5-C6-N1	5.05	123.53	121.00
1	2A	2277	G	OP1-P-OP2	5.05	127.17	119.60
32	2a	125	U	C6-N1-C2	-5.05	117.97	121.00
1	1A	992	C	C5-C6-N1	-5.05	118.48	121.00
1	1A	2356	C	C2-N1-C1'	-5.05	113.25	118.80
1	2A	185	U	C5-C6-N1	-5.05	120.18	122.70
1	2A	471	A	O5'-P-OP2	5.05	116.76	110.70
1	2A	2297	C	N1-C1'-C2'	-5.05	106.45	112.00
1	2A	2747	G	C6-C5-N7	-5.05	127.37	130.40
1	1A	73	A	N3-C4-C5	-5.05	123.27	126.80
1	1A	103	A	OP1-P-OP2	-5.05	112.03	119.60
1	1A	539	G	N1-C2-N3	-5.05	120.87	123.90
1	1A	579	G	OP1-P-OP2	5.05	127.17	119.60
1	1A	608	A	N7-C8-N9	5.05	116.32	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	668	G	OP1-P-OP2	-5.05	112.03	119.60
1	1A	715	G	C5-C6-O6	-5.05	125.57	128.60
1	1A	805	G	C4-C5-N7	5.05	112.82	110.80
1	1A	1091	G	C2-N3-C4	5.05	114.42	111.90
1	1A	1409	C	C5-C6-N1	-5.05	118.48	121.00
1	1A	2356	C	O5'-P-OP2	5.05	116.76	110.70
1	1A	2677	G	C4-C5-C6	-5.05	115.77	118.80
2	1B	63	G	C5-C6-O6	5.05	131.63	128.60
18	1W	90	ARG	NE-CZ-NH2	5.05	122.82	120.30
1	2A	1037	G	N3-C4-C5	5.05	131.12	128.60
1	2A	1617	C	OP1-P-OP2	-5.05	112.03	119.60
1	2A	2721	A	C2-N3-C4	-5.05	108.08	110.60
1	1A	349	G	N1-C6-O6	5.04	122.93	119.90
1	1A	433	C	N1-C2-N3	5.04	122.73	119.20
1	1A	986	C	N3-C2-O2	5.04	125.43	121.90
1	1A	1320	C	N1-C2-N3	5.04	122.73	119.20
1	1A	2091	U	C4-C5-C6	5.04	122.73	119.70
1	1A	2447	G	C4-C5-C6	5.04	121.83	118.80
1	1A	2553	G	C4-N9-C1'	5.04	133.06	126.50
32	1a	812	C	C5-C6-N1	5.04	123.52	121.00
1	2A	471	A	C8-N9-C4	5.04	107.82	105.80
1	2A	482	A	N9-C4-C5	-5.04	103.78	105.80
1	2A	1583	A	C5-C6-N1	5.04	120.22	117.70
1	2A	1840	G	N3-C2-N2	5.04	123.43	119.90
1	2A	2522	U	OP2-P-O3'	5.04	116.30	105.20
32	2a	428	G	C6-C5-N7	5.04	133.43	130.40
32	2a	1528	U	N3-C4-C5	5.04	117.63	114.60
1	1A	496	G	N9-C4-C5	5.04	107.42	105.40
1	1A	1618	A	N1-C2-N3	5.04	131.82	129.30
1	1A	2029	G	C6-N1-C2	5.04	128.13	125.10
1	1A	2070	G	C6-C5-N7	-5.04	127.37	130.40
32	1a	1512	U	C5-C6-N1	-5.04	120.18	122.70
1	2A	1561	G	N1-C2-N2	5.04	120.74	116.20
1	2A	1702	G	OP2-P-O3'	5.04	116.30	105.20
1	2A	2017	U	N3-C4-C5	-5.04	111.57	114.60
1	2A	2054	A	OP2-P-O3'	5.04	116.30	105.20
1	2A	2759	G	N1-C6-O6	5.04	122.93	119.90
1	2A	2824	C	C4-C5-C6	5.04	119.92	117.40
32	2a	353	A	OP2-P-O3'	5.04	116.29	105.20
32	2a	525	C	C5-C4-N4	-5.04	116.67	120.20
32	2a	946	A	C2-N3-C4	-5.04	108.08	110.60
1	1A	308	G	C8-N9-C4	-5.04	104.38	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	650	C	O5'-P-OP2	-5.04	101.16	105.70
1	1A	1035	U	C5-C6-N1	-5.04	120.18	122.70
1	1A	2080	G	OP1-P-OP2	5.04	127.16	119.60
1	1A	2881	C	OP1-P-OP2	5.04	127.16	119.60
2	1B	99	G	OP1-P-OP2	5.04	127.16	119.60
32	1a	1256	A	C8-N9-C4	-5.04	103.78	105.80
1	2A	758	C	N3-C4-C5	5.04	123.92	121.90
1	2A	2048	G	N7-C8-N9	5.04	115.62	113.10
32	2a	450	G	C8-N9-C4	5.04	108.42	106.40
1	1A	730	C	OP2-P-O3'	5.04	116.29	105.20
1	1A	1014	U	C4-C5-C6	5.04	122.72	119.70
1	1A	1204	A	OP1-P-OP2	5.04	127.16	119.60
1	1A	2453	A	N1-C2-N3	-5.04	126.78	129.30
1	1A	2685	G	C8-N9-C1'	5.04	133.55	127.00
1	1A	2810	A	C4-C5-N7	5.04	113.22	110.70
1	2A	972	G	OP1-P-O3'	5.04	116.29	105.20
1	2A	1234	U	N3-C2-O2	-5.04	118.67	122.20
1	1A	35	G	OP1-P-OP2	5.04	127.16	119.60
1	1A	446	G	N3-C4-C5	5.04	131.12	128.60
1	1A	575	A	C4-C5-C6	5.04	119.52	117.00
1	1A	1557	C	C2-N1-C1'	-5.04	113.26	118.80
1	1A	1650	G	C5-C6-N1	-5.04	108.98	111.50
1	1A	1933	G	O5'-P-OP1	-5.04	101.17	105.70
1	1A	2039	C	C6-N1-C2	-5.04	118.28	120.30
32	1a	34	C	N3-C2-O2	5.04	125.43	121.90
32	1a	715	A	O5'-P-OP1	-5.04	101.17	105.70
1	2A	55	G	C5-N7-C8	-5.04	101.78	104.30
1	2A	226	G	O4'-C1'-N9	5.04	112.23	108.20
1	2A	715	G	C8-N9-C4	-5.04	104.39	106.40
1	2A	1023	U	C5-C6-N1	-5.04	120.18	122.70
1	2A	2121	G	N3-C4-C5	-5.04	126.08	128.60
32	2a	998	G	N9-C4-C5	-5.04	103.38	105.40
32	2a	1462	G	C5-C6-N1	-5.04	108.98	111.50
1	1A	488	G	C8-N9-C4	-5.04	104.39	106.40
1	1A	1133	U	C2-N1-C1'	-5.04	111.66	117.70
1	1A	1452	A	C6-C5-N7	-5.04	128.77	132.30
1	1A	1574	C	OP2-P-O3'	5.04	116.28	105.20
1	1A	2529	G	O4'-C1'-N9	-5.04	104.17	108.20
1	1A	2607	G	N3-C4-C5	5.04	131.12	128.60
2	1B	102	A	C8-N9-C4	5.04	107.81	105.80
1	2A	2762	G	C8-N9-C4	5.04	108.42	106.40
32	2a	397	A	N3-C4-C5	-5.04	123.27	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1531	A	C4-C5-N7	5.04	113.22	110.70
1	1A	427	U	N1-C2-N3	-5.04	111.88	114.90
1	1A	1206	G	N3-C4-N9	5.04	129.02	126.00
1	1A	1810	A	C4-C5-C6	5.04	119.52	117.00
1	1A	1890	A	C5-C6-N6	5.04	127.73	123.70
1	1A	2001	A	C6-C5-N7	5.04	135.83	132.30
1	1A	2349	G	C5-C6-O6	5.04	131.62	128.60
1	1A	2585	U	O5'-P-OP1	-5.04	101.17	105.70
32	1a	812	C	C6-N1-C2	-5.04	118.29	120.30
32	1a	917	G	C8-N9-C4	-5.04	104.39	106.40
1	2A	363(B)	G	N3-C4-N9	5.04	129.02	126.00
1	2A	773	U	N1-C2-N3	5.04	117.92	114.90
1	2A	842	G	N1-C2-N3	5.04	126.92	123.90
1	2A	1239	G	C5-C6-O6	-5.04	125.58	128.60
1	2A	1359	A	C8-N9-C4	5.04	107.81	105.80
1	2A	2062	A	N9-C4-C5	-5.04	103.79	105.80
13	2R	114	VAL	CB-CA-C	-5.04	101.83	111.40
32	2a	500	G	O5'-P-OP2	-5.04	101.17	105.70
1	1A	995	C	N3-C2-O2	-5.03	118.38	121.90
1	1A	1176	G	P-O3'-C3'	5.03	125.74	119.70
1	1A	2244	U	C2-N3-C4	-5.03	123.98	127.00
1	1A	2422	A	N9-C4-C5	5.03	107.81	105.80
1	1A	2500	U	N1-C1'-C2'	-5.03	106.46	112.00
1	1A	2678	C	N3-C4-N4	-5.03	114.48	118.00
2	1B	101	G	C6-N1-C2	-5.03	122.08	125.10
32	1a	33	A	N7-C8-N9	-5.03	111.28	113.80
32	1a	231	G	O5'-P-OP2	-5.03	101.17	105.70
32	1a	773	G	C4-N9-C1'	-5.03	119.96	126.50
32	1a	1481	U	N1-C2-N3	5.03	117.92	114.90
1	2A	1494	A	C2-N3-C4	-5.03	108.08	110.60
1	2A	1609	A	C5-N7-C8	-5.03	101.38	103.90
32	2a	755	G	N1-C6-O6	5.03	122.92	119.90
32	2a	1068	G	C8-N9-C4	-5.03	104.39	106.40
1	1A	504	U	N3-C4-O4	5.03	122.92	119.40
1	1A	1379	A	N1-C2-N3	-5.03	126.78	129.30
1	1A	1436	G	C4-C5-N7	5.03	112.81	110.80
1	1A	2517	C	N3-C2-O2	5.03	125.42	121.90
32	1a	73	G	N3-C4-N9	-5.03	122.98	126.00
1	2A	195	A	P-O3'-C3'	5.03	125.74	119.70
1	2A	2498	C	N3-C4-C5	-5.03	119.89	121.90
1	2A	2623	G	C8-N9-C4	-5.03	104.39	106.40
1	2A	2789	C	C5-C4-N4	5.03	123.72	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	285	C	C2-N3-C4	-5.03	117.38	119.90
1	1A	768	G	N7-C8-N9	5.03	115.61	113.10
1	1A	1186	G	C5-N7-C8	5.03	106.82	104.30
1	1A	1297	C	OP1-P-O3'	5.03	116.27	105.20
1	1A	2506	U	OP2-P-O3'	5.03	116.27	105.20
1	1A	2680	C	N1-C2-O2	-5.03	115.88	118.90
32	1a	1525	G	C5-C6-O6	-5.03	125.58	128.60
1	2A	387	U	C5-C6-N1	-5.03	120.19	122.70
1	2A	786	C	C2-N1-C1'	-5.03	113.27	118.80
1	2A	851	U	C2-N3-C4	-5.03	123.98	127.00
1	2A	989	G	C4-C5-N7	5.03	112.81	110.80
32	2a	108	G	C6-C5-N7	-5.03	127.38	130.40
32	2a	753	A	N9-C4-C5	5.03	107.81	105.80
32	2a	1460	A	O5'-P-OP1	5.03	116.74	110.70
1	1A	479	A	N7-C8-N9	-5.03	111.29	113.80
1	1A	1928	A	C8-N9-C4	-5.03	103.79	105.80
32	1a	372	C	N1-C2-N3	-5.03	115.68	119.20
1	2A	1036	G	O5'-P-OP1	5.03	116.73	110.70
1	2A	2230	G	O5'-P-OP1	-5.03	101.17	105.70
32	2a	743	U	N3-C2-O2	-5.03	118.68	122.20
1	1A	395	U	N1-C2-N3	-5.03	111.88	114.90
1	1A	947	G	C5-N7-C8	-5.03	101.79	104.30
1	1A	1014	U	N1-C2-O2	-5.03	119.28	122.80
1	1A	1055	G	N3-C4-C5	-5.03	126.09	128.60
1	1A	1335	U	C5-C6-N1	-5.03	120.19	122.70
1	1A	1468	C	N1-C2-O2	-5.03	115.88	118.90
32	1a	427	U	C2-N1-C1'	5.03	123.73	117.70
32	1a	593	G	N1-C6-O6	5.03	122.92	119.90
32	1a	1486	G	N3-C4-C5	5.03	131.11	128.60
1	2A	464	U	C6-N1-C2	-5.03	117.98	121.00
1	2A	1248	G	O5'-P-OP2	-5.03	101.18	105.70
1	2A	1770	G	N3-C4-C5	-5.03	126.09	128.60
1	2A	2861	G	C5-C6-N1	-5.03	108.99	111.50
2	2B	15	A	C6-C5-N7	5.03	135.82	132.30
1	1A	1397	U	O5'-P-OP2	5.03	116.73	110.70
1	1A	1795	C	N1-C2-N3	-5.03	115.68	119.20
32	1a	818	G	C5-C6-O6	5.03	131.62	128.60
1	2A	123	G	O5'-P-OP2	-5.03	101.18	105.70
1	2A	501	A	C5-C6-N6	5.03	127.72	123.70
1	2A	1888	G	C4-C5-N7	5.03	112.81	110.80
1	2A	2010	G	C6-N1-C2	5.03	128.12	125.10
1	2A	2481	G	O4'-C1'-N9	5.03	112.22	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	594	G	N1-C6-O6	5.03	122.92	119.90
1	1A	719	C	N3-C4-C5	5.02	123.91	121.90
1	2A	2133	G	O4'-C1'-N9	5.02	112.22	108.20
1	2A	2587	A	C8-N9-C4	5.02	107.81	105.80
2	2B	78	A	N1-C6-N6	5.02	121.61	118.60
32	2a	1433	A	O5'-P-OP1	-5.02	101.18	105.70
1	1A	315	G	OP1-P-O3'	5.02	116.25	105.20
1	1A	1060	U	N1-C2-O2	5.02	126.32	122.80
1	1A	1994	C	C5-C6-N1	-5.02	118.49	121.00
1	1A	2004	G	C5-C6-N1	-5.02	108.99	111.50
1	1A	2365	G	O5'-P-OP2	-5.02	101.18	105.70
1	1A	2823	A	P-O3'-C3'	5.02	125.73	119.70
1	1A	2894	G	C4-N9-C1'	-5.02	119.97	126.50
2	1B	101	G	O5'-P-OP2	-5.02	101.18	105.70
32	1a	153	C	N1-C2-O2	5.02	121.91	118.90
32	1a	1077	G	N9-C1'-C2'	-5.02	106.47	112.00
1	2A	606	U	C5-C6-N1	-5.02	120.19	122.70
1	2A	620	G	C4-C5-N7	-5.02	108.79	110.80
1	2A	1937	A	C5-C6-N6	5.02	127.72	123.70
1	2A	2171	A	N1-C6-N6	5.02	121.61	118.60
1	2A	2661	G	N1-C6-O6	5.02	122.91	119.90
1	1A	148	C	C6-N1-C2	5.02	122.31	120.30
1	1A	880	G	N7-C8-N9	5.02	115.61	113.10
1	1A	2024	G	N1-C6-O6	5.02	122.91	119.90
32	1a	26	A	N1-C6-N6	-5.02	115.59	118.60
32	1a	810	C	OP1-P-O3'	5.02	116.25	105.20
1	2A	638	G	C8-N9-C4	-5.02	104.39	106.40
1	2A	2449	U	N3-C4-O4	5.02	122.92	119.40
1	1A	570	G	N9-C4-C5	5.02	107.41	105.40
1	1A	1549	C	O5'-P-OP2	5.02	116.72	110.70
1	1A	1832	C	C6-N1-C2	-5.02	118.29	120.30
1	1A	2013	A	C5-C6-N6	5.02	127.72	123.70
1	1A	2568	C	OP1-P-OP2	5.02	127.13	119.60
1	1A	2583	G	N3-C4-N9	-5.02	122.99	126.00
1	1A	2780	G	C4-C5-N7	-5.02	108.79	110.80
32	1a	585	G	N3-C4-N9	5.02	129.01	126.00
32	1a	1390	U	N3-C2-O2	5.02	125.71	122.20
32	1a	1438	G	C8-N9-C4	-5.02	104.39	106.40
1	2A	668	G	OP2-P-O3'	5.02	116.24	105.20
1	2A	682	G	N1-C6-O6	5.02	122.91	119.90
1	2A	2238	G	C2-N3-C4	5.02	114.41	111.90
1	1A	254	G	C4-C5-C6	5.02	121.81	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	351	G	O5'-P-OP2	5.02	116.72	110.70
1	1A	809	G	C4-C5-N7	5.02	112.81	110.80
1	1A	813	U	N3-C2-O2	-5.02	118.69	122.20
1	1A	1343	G	C4-C5-C6	5.02	121.81	118.80
1	1A	1792	G	C5-N7-C8	5.02	106.81	104.30
1	1A	1801	G	N1-C2-N2	5.02	120.72	116.20
1	1A	2229	C	N3-C4-C5	-5.02	119.89	121.90
1	1A	2239	G	P-O3'-C3'	5.02	125.72	119.70
1	1A	2576	G	C5-N7-C8	-5.02	101.79	104.30
1	1A	2765	A	OP1-P-OP2	5.02	127.13	119.60
32	1a	42	G	C8-N9-C4	5.02	108.41	106.40
1	2A	271(F)	C	C6-N1-C2	-5.02	118.29	120.30
1	2A	594	U	N1-C2-N3	5.02	117.91	114.90
1	2A	1108	U	C6-N1-C2	-5.02	117.99	121.00
1	2A	2634	G	O5'-P-OP2	-5.02	101.18	105.70
32	2a	354	G	C4-C5-N7	5.02	112.81	110.80
1	1A	834	C	C6-N1-C2	5.02	122.31	120.30
2	2B	81	G	N7-C8-N9	5.02	115.61	113.10
32	2a	1361	G	C8-N9-C4	-5.02	104.39	106.40
1	1A	583	G	O5'-P-OP2	-5.01	101.19	105.70
1	1A	1363	C	C6-N1-C1'	5.01	126.82	120.80
1	1A	1392	A	OP2-P-O3'	5.01	116.23	105.20
1	1A	1812	A	N3-C4-C5	-5.01	123.29	126.80
1	1A	1937	A	C5-C6-N6	5.01	127.71	123.70
1	1A	2263	C	P-O3'-C3'	-5.01	113.68	119.70
1	1A	2358	G	N1-C2-N2	5.01	120.71	116.20
1	1A	2641	G	O5'-P-OP1	-5.01	101.19	105.70
1	1A	2859	G	N7-C8-N9	-5.01	110.59	113.10
32	1a	696	A	C4-C5-C6	5.01	119.51	117.00
32	1a	779	C	OP1-P-O3'	5.01	116.23	105.20
32	1a	1003	G	N3-C4-C5	-5.01	126.09	128.60
32	1a	1340	A	C5-C6-N1	-5.01	115.19	117.70
1	2A	1688	U	C6-N1-C1'	5.01	128.22	121.20
1	2A	2356	C	N1-C2-N3	5.01	122.71	119.20
1	2A	2378	A	C5-C6-N6	-5.01	119.69	123.70
32	2a	640	A	N1-C6-N6	-5.01	115.59	118.60
1	1A	1006	C	C6-N1-C2	-5.01	118.30	120.30
1	1A	1613	G	C5-C6-N1	-5.01	108.99	111.50
1	1A	2049	G	C8-N9-C4	5.01	108.41	106.40
32	1a	1053	G	N1-C6-O6	5.01	122.91	119.90
1	2A	496	G	N1-C2-N3	5.01	126.91	123.90
1	2A	2342	C	C6-N1-C2	-5.01	118.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2514	U	C2-N1-C1'	-5.01	111.68	117.70
1	1A	641	C	C6-N1-C2	-5.01	118.30	120.30
1	1A	1099	G	C5-C6-O6	-5.01	125.59	128.60
1	1A	1706	U	C5-C6-N1	-5.01	120.19	122.70
1	1A	2206	G	N3-C4-C5	5.01	131.11	128.60
1	1A	2784	C	C2-N1-C1'	5.01	124.31	118.80
4	1E	79	ARG	NE-CZ-NH1	-5.01	117.79	120.30
32	1a	685	G	C5-C6-N1	-5.01	108.99	111.50
32	1a	1030(A)	G	O4'-C1'-N9	5.01	112.21	108.20
32	1a	1513	A	OP2-P-O3'	5.01	116.23	105.20
1	2A	1304	C	N3-C4-C5	5.01	123.91	121.90
1	2A	1512	U	N3-C2-O2	5.01	125.71	122.20
1	2A	1832	C	C6-N1-C2	5.01	122.31	120.30
1	2A	1983	C	OP1-P-OP2	5.01	127.12	119.60
1	2A	2584	U	N3-C2-O2	-5.01	118.69	122.20
32	2a	251	G	N9-C4-C5	-5.01	103.39	105.40
1	1A	949	C	N1-C2-N3	5.01	122.71	119.20
1	1A	2677	G	N1-C6-O6	-5.01	116.89	119.90
1	2A	20	C	N3-C4-C5	-5.01	119.90	121.90
1	2A	365	C	N3-C4-N4	5.01	121.51	118.00
1	2A	1124	C	OP1-P-OP2	5.01	127.11	119.60
1	2A	1331	A	C4-C5-N7	-5.01	108.20	110.70
1	2A	1770	G	C4-C5-N7	-5.01	108.80	110.80
1	2A	2508	G	OP1-P-OP2	-5.01	112.08	119.60
32	2a	700	G	N1-C6-O6	5.01	122.91	119.90
32	2a	1234	C	C6-N1-C2	5.01	122.30	120.30
32	2a	1420	C	N3-C4-C5	-5.01	119.90	121.90
1	1A	530	G	C6-C5-N7	5.01	133.41	130.40
1	1A	681	G	OP2-P-O3'	5.01	116.22	105.20
1	1A	1579	A	N1-C6-N6	5.01	121.61	118.60
1	1A	1864	U	C5-C4-O4	5.01	128.91	125.90
1	1A	2239	G	O4'-C1'-N9	-5.01	104.19	108.20
1	1A	2493	U	N3-C4-O4	-5.01	115.89	119.40
32	1a	1530	G	C5-N7-C8	-5.01	101.80	104.30
1	2A	12	U	C6-N1-C1'	-5.01	114.19	121.20
1	2A	252	G	OP1-P-O3'	5.01	116.22	105.20
1	2A	1064	C	C6-N1-C2	-5.01	118.30	120.30
1	2A	2613	U	N1-C2-O2	5.01	126.31	122.80
2	2B	65	C	C6-N1-C2	-5.01	118.30	120.30
32	2a	273	A	C8-N9-C4	5.01	107.80	105.80
32	2a	1486	G	N9-C4-C5	-5.01	103.40	105.40
1	1A	60	G	C5-N7-C8	5.01	106.80	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	95	G	N7-C8-N9	5.01	115.60	113.10
1	1A	1374	G	C5-C6-N1	-5.01	109.00	111.50
1	1A	1428	C	O5'-P-OP1	-5.01	101.19	105.70
1	1A	1926	U	O5'-P-OP2	-5.01	101.19	105.70
1	1A	2472	G	C5-C6-N1	5.01	114.00	111.50
1	1A	2504	U	C5-C6-N1	5.01	125.20	122.70
1	1A	2677	G	OP2-P-O3'	5.01	116.21	105.20
32	1a	260	G	C5-C6-N1	-5.01	109.00	111.50
32	1a	339	C	C2-N1-C1'	-5.01	113.29	118.80
32	1a	728	A	C5-N7-C8	-5.01	101.40	103.90
32	1a	1525	G	N3-C2-N2	5.01	123.41	119.90
1	2A	274	G	N3-C4-C5	-5.01	126.10	128.60
1	2A	559	G	C5-C6-O6	-5.01	125.60	128.60
1	2A	678	C	C6-N1-C2	5.01	122.30	120.30
1	2A	1031	G	C5-C6-O6	-5.01	125.60	128.60
1	2A	1351	C	N1-C2-N3	5.01	122.70	119.20
1	2A	2206	G	N3-C4-N9	-5.01	123.00	126.00
1	2A	2763	G	N9-C4-C5	-5.01	103.40	105.40
2	2B	56	G	C8-N9-C4	-5.01	104.40	106.40
32	2a	1033	G	C8-N9-C4	-5.01	104.40	106.40
1	1A	774	A	O5'-P-OP1	5.00	116.71	110.70
1	1A	990	A	C8-N9-C4	-5.00	103.80	105.80
1	1A	1025	G	N3-C4-N9	-5.00	123.00	126.00
1	1A	590	A	N1-C6-N6	-5.00	115.60	118.60
1	1A	2294	C	C2-N1-C1'	5.00	124.30	118.80
1	1A	2492	U	N1-C2-O2	5.00	126.30	122.80
1	1A	2509	G	O5'-P-OP2	-5.00	101.20	105.70
1	1A	2522	U	C6-N1-C2	5.00	124.00	121.00
1	1A	2622	C	C5-C4-N4	-5.00	116.70	120.20
2	1B	101	G	O5'-P-OP1	5.00	116.70	110.70
4	1E	144	ARG	NE-CZ-NH2	-5.00	117.80	120.30
32	1a	982	U	C2-N1-C1'	-5.00	111.69	117.70
1	2A	1162	G	OP1-P-O3'	5.00	116.21	105.20
1	2A	1334	G	C5-C6-O6	5.00	131.60	128.60
1	2A	1410	G	N1-C2-N3	5.00	126.90	123.90
1	2A	1690	A	N9-C4-C5	-5.00	103.80	105.80
1	2A	2861	G	N1-C6-O6	5.00	122.90	119.90
2	2B	61	G	N1-C6-O6	5.00	122.90	119.90
32	2a	899	C	C6-N1-C2	5.00	122.30	120.30
32	2a	998	G	C8-N9-C1'	-5.00	120.50	127.00
1	1A	441	U	N3-C2-O2	5.00	125.70	122.20
1	1A	645	C	C2-N3-C4	5.00	122.40	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1425	G	OP1-P-OP2	5.00	127.10	119.60
1	1A	1488	G	OP1-P-O3'	5.00	116.20	105.20
1	1A	2056	G	N7-C8-N9	5.00	115.60	113.10
1	1A	2219	G	C5-C6-N1	-5.00	109.00	111.50
1	1A	2392	A	O5'-P-OP1	-5.00	101.20	105.70
1	1A	2669	G	N3-C4-C5	5.00	131.10	128.60
2	1B	67	G	O5'-P-OP1	-5.00	101.20	105.70
21	1Z	123	ASP	CB-CG-OD1	5.00	122.80	118.30
32	1a	326	G	C5-C6-O6	5.00	131.60	128.60
1	2A	141	A	C4-C5-N7	5.00	113.20	110.70
1	2A	198	C	OP2-P-O3'	5.00	116.20	105.20
1	2A	271(B)	C	C6-N1-C2	-5.00	118.30	120.30
1	2A	325	G	C8-N9-C4	5.00	108.40	106.40
1	2A	592	G	C8-N9-C4	-5.00	104.40	106.40
1	2A	967	C	C2-N1-C1'	-5.00	113.30	118.80
1	2A	1661	G	C6-C5-N7	-5.00	127.40	130.40
1	2A	1702	G	C2-N3-C4	5.00	114.40	111.90

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	1E	11	MET	Peptide
14	1S	58	LEU	Peptide
15	1T	128	GLU	Peptide
19	1X	93	GLU	Peptide
44	1m	113	PRO	Peptide
53	1y	20	PRO	Peptide
4	2E	11	MET	Peptide
14	2S	58	LEU	Peptide
15	2T	128	GLU	Peptide
19	2X	93	GLU	Peptide
33	2b	11	LEU	Peptide
44	2m	113	PRO	Peptide

## 5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/275 (99%)	256 (94%)	17 (6%)	0	100	100
3	2D	273/275 (99%)	257 (94%)	14 (5%)	2 (1%)	22	61
4	1E	202/204 (99%)	189 (94%)	12 (6%)	1 (0%)	29	67
4	2E	202/204 (99%)	189 (94%)	12 (6%)	1 (0%)	29	67
5	1F	201/203 (99%)	187 (93%)	11 (6%)	3 (2%)	10	44
5	2F	201/203 (99%)	186 (92%)	13 (6%)	2 (1%)	15	54
6	1G	179/181 (99%)	155 (87%)	16 (9%)	8 (4%)	2	18
6	2G	179/181 (99%)	152 (85%)	20 (11%)	7 (4%)	3	22
7	1H	172/174 (99%)	156 (91%)	15 (9%)	1 (1%)	25	64
7	2H	172/174 (99%)	153 (89%)	17 (10%)	2 (1%)	13	49
8	1I	145/147 (99%)	118 (81%)	24 (17%)	3 (2%)	7	37
8	2I	145/147 (99%)	116 (80%)	25 (17%)	4 (3%)	5	29
9	1N	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
9	2N	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
10	1O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	19	58
10	2O	120/122 (98%)	113 (94%)	4 (3%)	3 (2%)	5	32
11	1P	147/149 (99%)	125 (85%)	21 (14%)	1 (1%)	22	61
11	2P	147/149 (99%)	130 (88%)	15 (10%)	2 (1%)	11	46
12	1Q	139/141 (99%)	125 (90%)	14 (10%)	0	100	100
12	2Q	139/141 (99%)	125 (90%)	12 (9%)	2 (1%)	11	46
13	1R	116/118 (98%)	98 (84%)	16 (14%)	2 (2%)	9	42
13	2R	116/118 (98%)	98 (84%)	17 (15%)	1 (1%)	17	56
14	1S	108/110 (98%)	96 (89%)	12 (11%)	0	100	100
14	2S	108/110 (98%)	94 (87%)	14 (13%)	0	100	100
15	1T	129/131 (98%)	122 (95%)	6 (5%)	1 (1%)	19	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/131 (98%)	120 (93%)	8 (6%)	1 (1%)	19	58
16	1U	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
16	2U	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	91 (92%)	8 (8%)	0	100	100
17	2V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	15	54
18	1W	110/112 (98%)	100 (91%)	10 (9%)	0	100	100
18	2W	110/112 (98%)	104 (94%)	6 (6%)	0	100	100
19	1X	93/95 (98%)	90 (97%)	2 (2%)	1 (1%)	14	51
19	2X	93/95 (98%)	88 (95%)	5 (5%)	0	100	100
20	1Y	105/107 (98%)	93 (89%)	11 (10%)	1 (1%)	15	54
20	2Y	105/107 (98%)	93 (89%)	11 (10%)	1 (1%)	15	54
21	1Z	201/203 (99%)	170 (85%)	30 (15%)	1 (0%)	29	67
21	2Z	201/203 (99%)	174 (87%)	26 (13%)	1 (0%)	29	67
22	10	75/77 (97%)	67 (89%)	8 (11%)	0	100	100
22	20	75/77 (97%)	67 (89%)	8 (11%)	0	100	100
23	11	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
23	21	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
24	12	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
24	22	68/70 (97%)	63 (93%)	5 (7%)	0	100	100
25	13	57/59 (97%)	52 (91%)	4 (7%)	1 (2%)	8	41
25	23	57/59 (97%)	51 (90%)	6 (10%)	0	100	100
26	14	67/69 (97%)	52 (78%)	11 (16%)	4 (6%)	1	12
26	24	67/69 (97%)	51 (76%)	12 (18%)	4 (6%)	1	12
27	15	57/59 (97%)	53 (93%)	4 (7%)	0	100	100
27	25	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
28	16	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
28	26	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
29	17	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
29	27	46/48 (96%)	43 (94%)	3 (6%)	0	100	100
30	18	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
30	28	62/64 (97%)	59 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/231 (99%)	174 (76%)	39 (17%)	16 (7%)	1	8
33	2b	229/231 (99%)	174 (76%)	40 (18%)	15 (7%)	1	9
34	1c	204/206 (99%)	175 (86%)	26 (13%)	3 (2%)	10	44
34	2c	204/206 (99%)	173 (85%)	27 (13%)	4 (2%)	7	38
35	1d	206/208 (99%)	176 (85%)	24 (12%)	6 (3%)	4	28
35	2d	206/208 (99%)	172 (84%)	29 (14%)	5 (2%)	6	34
36	1e	146/148 (99%)	124 (85%)	20 (14%)	2 (1%)	11	46
36	2e	146/148 (99%)	125 (86%)	20 (14%)	1 (1%)	22	61
37	1f	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	15	54
37	2f	98/100 (98%)	87 (89%)	10 (10%)	1 (1%)	15	54
38	1g	153/155 (99%)	133 (87%)	18 (12%)	2 (1%)	12	47
38	2g	153/155 (99%)	132 (86%)	18 (12%)	3 (2%)	7	38
39	1h	135/137 (98%)	122 (90%)	13 (10%)	0	100	100
39	2h	135/137 (98%)	123 (91%)	12 (9%)	0	100	100
40	1i	125/127 (98%)	105 (84%)	16 (13%)	4 (3%)	4	26
40	2i	125/127 (98%)	105 (84%)	15 (12%)	5 (4%)	3	21
41	1j	95/97 (98%)	76 (80%)	17 (18%)	2 (2%)	7	37
41	2j	95/97 (98%)	72 (76%)	20 (21%)	3 (3%)	4	26
42	1k	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
42	2k	112/114 (98%)	97 (87%)	14 (12%)	1 (1%)	17	56
43	1l	119/122 (98%)	100 (84%)	19 (16%)	0	100	100
43	2l	119/122 (98%)	104 (87%)	15 (13%)	0	100	100
44	1m	114/116 (98%)	99 (87%)	13 (11%)	2 (2%)	8	41
44	2m	114/116 (98%)	101 (89%)	10 (9%)	3 (3%)	5	31
45	1n	58/60 (97%)	52 (90%)	5 (9%)	1 (2%)	9	42
45	2n	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
46	1o	86/88 (98%)	76 (88%)	9 (10%)	1 (1%)	13	49
46	2o	86/88 (98%)	79 (92%)	6 (7%)	1 (1%)	13	49
47	1p	80/82 (98%)	59 (74%)	19 (24%)	2 (2%)	5	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/82 (98%)	60 (75%)	19 (24%)	1 (1%)	12	47
48	1q	97/99 (98%)	87 (90%)	7 (7%)	3 (3%)	4	26
48	2q	97/99 (98%)	85 (88%)	9 (9%)	3 (3%)	4	26
49	1r	66/68 (97%)	55 (83%)	9 (14%)	2 (3%)	4	28
49	2r	66/68 (97%)	56 (85%)	8 (12%)	2 (3%)	4	28
50	1s	81/83 (98%)	74 (91%)	6 (7%)	1 (1%)	13	49
50	2s	81/83 (98%)	71 (88%)	9 (11%)	1 (1%)	13	49
51	1t	94/96 (98%)	74 (79%)	16 (17%)	4 (4%)	2	20
51	2t	94/96 (98%)	74 (79%)	16 (17%)	4 (4%)	2	20
52	1u	21/23 (91%)	15 (71%)	5 (24%)	1 (5%)	2	17
52	2u	21/23 (91%)	17 (81%)	3 (14%)	1 (5%)	2	17
53	1y	20/22 (91%)	12 (60%)	4 (20%)	4 (20%)	0	0
54	1z	95/97 (98%)	89 (94%)	5 (5%)	1 (1%)	14	51
54	2z	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
All	All	11656/11860 (98%)	10281 (88%)	1200 (10%)	175 (2%)	10	44

All (175) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	47	LYS
6	1G	126	ASP
20	1Y	92	ASN
21	1Z	31	ARG
26	14	44	THR
26	14	55	ARG
33	1b	17	PHE
33	1b	127	ILE
33	1b	155	LEU
33	1b	204	ASN
35	1d	129	ASN
37	1f	40	VAL
38	1g	33	ASP
40	1i	96	LEU
41	1j	79	ARG
44	1m	12	ASN
44	1m	113	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
48	1q	34	LYS
49	1r	25	THR
49	1r	36	ASN
51	1t	71	THR
52	1u	3	LYS
5	2F	130	ALA
6	2G	47	LYS
6	2G	50	ALA
6	2G	126	ASP
20	2Y	92	ASN
21	2Z	31	ARG
26	24	44	THR
26	24	49	PHE
26	24	55	ARG
33	2b	8	LYS
33	2b	9	GLU
33	2b	17	PHE
33	2b	126	GLU
33	2b	127	ILE
33	2b	155	LEU
33	2b	204	ASN
35	2d	129	ASN
37	2f	40	VAL
38	2g	33	ASP
41	2j	79	ARG
44	2m	113	PRO
49	2r	25	THR
49	2r	36	ASN
51	2t	71	THR
51	2t	95	ALA
52	2u	3	LYS
6	1G	43	LEU
6	1G	49	ASP
6	1G	50	ALA
6	1G	78	SER
6	1G	81	LYS
8	1I	16	GLY
10	1O	5	GLN
19	1X	19	ALA
26	14	45	GLY
26	14	49	PHE
33	1b	8	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
33	1b	10	LEU
33	1b	80	ILE
33	1b	83	MET
34	1c	26	LYS
34	1c	91	LEU
35	1d	171	GLY
36	1e	140	ARG
38	1g	4	ARG
40	1i	70	LYS
46	1o	86	GLY
50	1s	27	GLU
51	1t	67	ALA
51	1t	95	ALA
53	1y	18	ARG
6	2G	43	LEU
6	2G	81	LYS
8	2I	16	GLY
10	2O	5	GLN
33	2b	10	LEU
33	2b	80	ILE
34	2c	26	LYS
34	2c	91	LEU
35	2d	171	GLY
40	2i	44	VAL
40	2i	70	LYS
40	2i	96	LEU
44	2m	12	ASN
46	2o	86	GLY
4	1E	52	LEU
8	1I	73	GLU
15	1T	37	GLY
33	1b	110	GLN
40	1i	44	VAL
47	1p	52	ASP
48	1q	68	ARG
53	1y	4	ARG
53	1y	17	PRO
3	2D	11	PRO
4	2E	52	LEU
10	2O	26	LYS
15	2T	37	GLY
33	2b	124	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	2e	140	ARG
38	2g	4	ARG
48	2q	34	LYS
48	2q	68	ARG
51	2t	67	ALA
33	1b	9	GLU
33	1b	126	GLU
48	1q	49	GLU
51	1t	100	ILE
53	1y	21	PRO
33	2b	83	MET
33	2b	105	PHE
35	2d	179	GLU
41	2j	77	PRO
47	2p	52	ASP
51	2t	100	ILE
5	1F	160	ASN
11	1P	101	VAL
13	1R	3	HIS
33	1b	105	PHE
33	1b	131	PRO
33	1b	154	LEU
34	1c	84	ILE
35	1d	151	LYS
35	1d	164	ALA
54	1z	29	LYS
3	2D	30	GLU
6	2G	49	ASP
8	2I	103	ARG
10	2O	29	ASN
12	2Q	59	ARG
12	2Q	140	ALA
33	2b	110	GLN
38	2g	97	GLN
40	2i	53	VAL
44	2m	36	LYS
48	2q	49	GLU
50	2s	27	GLU
5	1F	161	GLU
13	1R	45	ARG
33	1b	227	GLY
45	1n	52	GLN

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Mol	Chain	Res	Type
7	2H	76	VAL
13	2R	53	HIS
26	24	45	GLY
33	2b	131	PRO
33	2b	227	GLY
34	2c	36	ASP
34	2c	84	ILE
35	2d	42	GLN
40	2i	127	LYS
42	2k	100	ALA
7	1H	76	VAL
8	1I	15	VAL
40	1i	53	VAL
11	2P	101	VAL
33	1b	124	SER
5	2F	25	PRO
8	2I	15	VAL
35	2d	37	PRO
25	13	41	PRO
6	2G	32	PRO
6	1G	32	PRO
35	1d	37	PRO
36	1e	96	PRO
41	1j	77	PRO
7	2H	126	PRO
8	2I	119	PRO
17	2V	79	VAL
35	1d	5	ILE
47	1p	46	PRO
11	2P	37	GLY
41	2j	36	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	214/217 (99%)	188 (88%)	26 (12%)	5	22
3	2D	214/217 (99%)	191 (89%)	23 (11%)	6	27
4	1E	164/165 (99%)	143 (87%)	21 (13%)	4	20
4	2E	164/165 (99%)	146 (89%)	18 (11%)	6	26
5	1F	160/161 (99%)	132 (82%)	28 (18%)	2	9
5	2F	160/161 (99%)	139 (87%)	21 (13%)	4	19
6	1G	144/155 (93%)	127 (88%)	17 (12%)	5	23
6	2G	144/155 (93%)	132 (92%)	12 (8%)	11	40
7	1H	144/145 (99%)	134 (93%)	10 (7%)	15	49
7	2H	144/145 (99%)	134 (93%)	10 (7%)	15	49
8	1I	111/123 (90%)	87 (78%)	24 (22%)	1	5
8	2I	111/123 (90%)	91 (82%)	20 (18%)	1	9
9	1N	119/119 (100%)	103 (87%)	16 (13%)	4	18
9	2N	119/119 (100%)	102 (86%)	17 (14%)	3	15
10	1O	100/100 (100%)	90 (90%)	10 (10%)	7	30
10	2O	100/100 (100%)	93 (93%)	7 (7%)	15	48
11	1P	115/116 (99%)	102 (89%)	13 (11%)	6	25
11	2P	115/116 (99%)	103 (90%)	12 (10%)	7	28
12	1Q	111/111 (100%)	100 (90%)	11 (10%)	8	30
12	2Q	111/111 (100%)	100 (90%)	11 (10%)	8	30
13	1R	101/101 (100%)	84 (83%)	17 (17%)	2	10
13	2R	101/101 (100%)	88 (87%)	13 (13%)	4	19
14	1S	87/87 (100%)	74 (85%)	13 (15%)	3	14
14	2S	87/87 (100%)	77 (88%)	10 (12%)	5	24
15	1T	115/115 (100%)	104 (90%)	11 (10%)	8	32
15	2T	115/115 (100%)	107 (93%)	8 (7%)	15	48
16	1U	93/93 (100%)	80 (86%)	13 (14%)	3	16
16	2U	93/93 (100%)	81 (87%)	12 (13%)	4	19
17	1V	81/82 (99%)	69 (85%)	12 (15%)	3	14
17	2V	81/82 (99%)	74 (91%)	7 (9%)	10	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	1W	90/91 (99%)	79 (88%)	11 (12%)	5	22
18	2W	90/91 (99%)	77 (86%)	13 (14%)	3	15
19	1X	77/77 (100%)	74 (96%)	3 (4%)	32	67
19	2X	77/77 (100%)	72 (94%)	5 (6%)	17	51
20	1Y	86/88 (98%)	75 (87%)	11 (13%)	4	20
20	2Y	86/88 (98%)	76 (88%)	10 (12%)	5	24
21	1Z	169/176 (96%)	147 (87%)	22 (13%)	4	19
21	2Z	169/176 (96%)	147 (87%)	22 (13%)	4	19
22	10	61/62 (98%)	60 (98%)	1 (2%)	62	84
22	20	61/62 (98%)	58 (95%)	3 (5%)	25	61
23	11	79/82 (96%)	72 (91%)	7 (9%)	9	35
23	21	79/82 (96%)	74 (94%)	5 (6%)	18	52
24	12	65/66 (98%)	59 (91%)	6 (9%)	9	33
24	22	65/66 (98%)	60 (92%)	5 (8%)	13	44
25	13	51/51 (100%)	41 (80%)	10 (20%)	1	7
25	23	51/51 (100%)	44 (86%)	7 (14%)	3	17
26	14	58/62 (94%)	48 (83%)	10 (17%)	2	10
26	24	58/62 (94%)	49 (84%)	9 (16%)	2	12
27	15	51/51 (100%)	45 (88%)	6 (12%)	5	23
27	25	51/51 (100%)	46 (90%)	5 (10%)	8	31
28	16	51/51 (100%)	43 (84%)	8 (16%)	2	12
28	26	51/51 (100%)	46 (90%)	5 (10%)	8	31
29	17	41/41 (100%)	34 (83%)	7 (17%)	2	10
29	27	41/41 (100%)	34 (83%)	7 (17%)	2	10
30	18	54/54 (100%)	49 (91%)	5 (9%)	9	33
30	28	54/54 (100%)	49 (91%)	5 (9%)	9	33
31	19	34/34 (100%)	30 (88%)	4 (12%)	5	23
31	29	34/34 (100%)	30 (88%)	4 (12%)	5	23
33	1b	191/199 (96%)	163 (85%)	28 (15%)	3	14
33	2b	191/199 (96%)	159 (83%)	32 (17%)	2	10
34	1c	144/160 (90%)	128 (89%)	16 (11%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	2c	144/160 (90%)	133 (92%)	11 (8%)	13	45
35	1d	171/180 (95%)	143 (84%)	28 (16%)	2	11
35	2d	171/180 (95%)	148 (86%)	23 (14%)	4	18
36	1e	114/114 (100%)	105 (92%)	9 (8%)	12	43
36	2e	114/114 (100%)	103 (90%)	11 (10%)	8	32
37	1f	85/90 (94%)	78 (92%)	7 (8%)	11	41
37	2f	85/90 (94%)	80 (94%)	5 (6%)	19	54
38	1g	120/126 (95%)	110 (92%)	10 (8%)	11	40
38	2g	120/126 (95%)	112 (93%)	8 (7%)	16	50
39	1h	116/118 (98%)	106 (91%)	10 (9%)	10	38
39	2h	116/118 (98%)	107 (92%)	9 (8%)	12	43
40	1i	91/98 (93%)	74 (81%)	17 (19%)	1	8
40	2i	91/98 (93%)	77 (85%)	14 (15%)	2	13
41	1j	68/87 (78%)	62 (91%)	6 (9%)	10	36
41	2j	68/87 (78%)	60 (88%)	8 (12%)	5	23
42	1k	83/86 (96%)	77 (93%)	6 (7%)	14	47
42	2k	83/86 (96%)	77 (93%)	6 (7%)	14	47
43	1l	96/102 (94%)	88 (92%)	8 (8%)	11	40
43	2l	96/102 (94%)	89 (93%)	7 (7%)	14	46
44	1m	90/94 (96%)	83 (92%)	7 (8%)	12	43
44	2m	90/94 (96%)	82 (91%)	8 (9%)	9	35
45	1n	49/49 (100%)	42 (86%)	7 (14%)	3	15
45	2n	49/49 (100%)	42 (86%)	7 (14%)	3	15
46	1o	78/79 (99%)	75 (96%)	3 (4%)	33	67
46	2o	78/79 (99%)	75 (96%)	3 (4%)	33	67
47	1p	69/71 (97%)	55 (80%)	14 (20%)	1	6
47	2p	69/71 (97%)	56 (81%)	13 (19%)	1	8
48	1q	94/94 (100%)	88 (94%)	6 (6%)	17	52
48	2q	94/94 (100%)	89 (95%)	5 (5%)	22	58
49	1r	59/59 (100%)	54 (92%)	5 (8%)	10	38
49	2r	59/59 (100%)	54 (92%)	5 (8%)	10	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	1s	68/72 (94%)	61 (90%)	7 (10%)	7	29
50	2s	68/72 (94%)	61 (90%)	7 (10%)	7	29
51	1t	71/74 (96%)	63 (89%)	8 (11%)	6	25
51	2t	71/74 (96%)	64 (90%)	7 (10%)	8	30
52	1u	18/18 (100%)	16 (89%)	2 (11%)	6	25
52	2u	18/18 (100%)	17 (94%)	1 (6%)	21	57
53	1y	16/21 (76%)	10 (62%)	6 (38%)	0	0
54	1z	82/83 (99%)	80 (98%)	2 (2%)	49	77
54	2z	82/83 (99%)	80 (98%)	2 (2%)	49	77
All	All	9582/9879 (97%)	8519 (89%)	1063 (11%)	6	25

All (1063) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	7	LYS
3	1D	10	THR
3	1D	12	SER
3	1D	13	ARG
3	1D	18	VAL
3	1D	37	LEU
3	1D	54	ARG
3	1D	61	LEU
3	1D	69	ARG
3	1D	94	LEU
3	1D	103	ARG
3	1D	104	TYR
3	1D	111	LEU
3	1D	138	VAL
3	1D	141	VAL
3	1D	142	VAL
3	1D	164	GLN
3	1D	169	GLU
3	1D	181	GLU
3	1D	200	ASP
3	1D	212	SER
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	253	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	1D	259	THR
4	1E	7	VAL
4	1E	9	VAL
4	1E	34	VAL
4	1E	45	THR
4	1E	47	VAL
4	1E	49	LEU
4	1E	64	LYS
4	1E	73	GLU
4	1E	77	ILE
4	1E	87	GLU
4	1E	89	ASP
4	1E	93	VAL
4	1E	113	PHE
4	1E	116	VAL
4	1E	119	ARG
4	1E	140	SER
4	1E	144	ARG
4	1E	175	VAL
4	1E	178	GLU
4	1E	181	LEU
4	1E	182	LEU
5	1F	7	TYR
5	1F	17	ARG
5	1F	24	LEU
5	1F	27	GLU
5	1F	33	LEU
5	1F	38	ARG
5	1F	53	THR
5	1F	74	ARG
5	1F	77	ASP
5	1F	78	ILE
5	1F	82	ILE
5	1F	88	VAL
5	1F	110	LEU
5	1F	125	LEU
5	1F	132	VAL
5	1F	137	LYS
5	1F	144	LYS
5	1F	148	LEU
5	1F	158	THR
5	1F	161	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	1F	162	LEU
5	1F	170	LEU
5	1F	191	ARG
5	1F	192	LEU
5	1F	195	ASP
5	1F	196	LEU
5	1F	197	ASP
5	1F	201	VAL
6	1G	7	LEU
6	1G	28	VAL
6	1G	31	VAL
6	1G	43	LEU
6	1G	49	ASP
6	1G	52	ILE
6	1G	53	LEU
6	1G	79	ASN
6	1G	81	LYS
6	1G	126	ASP
6	1G	139	LEU
6	1G	146	TYR
6	1G	150	ASP
6	1G	159	VAL
6	1G	161	THR
6	1G	162	THR
6	1G	165	THR
7	1H	3	ARG
7	1H	15	VAL
7	1H	24	VAL
7	1H	59	ARG
7	1H	84	SER
7	1H	85	LYS
7	1H	92	ILE
7	1H	129	THR
7	1H	133	VAL
7	1H	136	ILE
8	1I	3	VAL
8	1I	12	LEU
8	1I	19	VAL
8	1I	20	ASP
8	1I	35	LEU
8	1I	38	LEU
8	1I	42	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	1I	44	LEU
8	1I	47	LEU
8	1I	57	ARG
8	1I	60	GLU
8	1I	61	ARG
8	1I	64	GLU
8	1I	75	LEU
8	1I	78	THR
8	1I	82	ARG
8	1I	85	GLU
8	1I	92	VAL
8	1I	93	THR
8	1I	109	ILE
8	1I	116	LEU
8	1I	133	HIS
8	1I	140	LEU
8	1I	144	VAL
9	1N	1	MET
9	1N	5	VAL
9	1N	10	GLU
9	1N	32	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	55	VAL
9	1N	58	ASP
9	1N	61	ARG
9	1N	62	VAL
9	1N	63	THR
9	1N	65	LYS
9	1N	68	GLU
9	1N	87	LEU
9	1N	97	ARG
9	1N	99	LEU
10	1O	8	LEU
10	1O	23	ARG
10	1O	42	SER
10	1O	65	THR
10	1O	69	ILE
10	1O	82	ASN
10	1O	96	THR
10	1O	98	VAL
10	1O	109	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	1O	112	MET
11	1P	15	ARG
11	1P	18	ARG
11	1P	30	THR
11	1P	42	SER
11	1P	58	THR
11	1P	59	LEU
11	1P	65	ARG
11	1P	70	GLN
11	1P	90	ARG
11	1P	95	VAL
11	1P	125	VAL
11	1P	148	LEU
11	1P	149	GLU
12	1Q	1	MET
12	1Q	5	ARG
12	1Q	7	MET
12	1Q	8	LYS
12	1Q	17	LEU
12	1Q	18	LYS
12	1Q	35	VAL
12	1Q	59	ARG
12	1Q	75	THR
12	1Q	79	LEU
12	1Q	110	THR
13	1R	6	SER
13	1R	8	ARG
13	1R	17	ARG
13	1R	23	ASN
13	1R	29	LEU
13	1R	30	THR
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	75	LEU
13	1R	86	ARG
13	1R	91	GLN
13	1R	100	LEU
13	1R	111	LEU
13	1R	114	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	1S	14	VAL
14	1S	17	ARG
14	1S	21	THR
14	1S	23	ARG
14	1S	35	ILE
14	1S	36	TYR
14	1S	43	GLU
14	1S	46	VAL
14	1S	49	VAL
14	1S	50	SER
14	1S	59	LYS
14	1S	85	VAL
14	1S	110	LEU
15	1T	17	THR
15	1T	34	VAL
15	1T	49	VAL
15	1T	57	PHE
15	1T	59	THR
15	1T	74	ARG
15	1T	78	LEU
15	1T	96	ARG
15	1T	108	ARG
15	1T	120	ARG
15	1T	128	GLU
16	1U	5	LYS
16	1U	8	VAL
16	1U	17	ILE
16	1U	27	LEU
16	1U	30	LYS
16	1U	59	ARG
16	1U	74	LEU
16	1U	77	SER
16	1U	83	LEU
16	1U	95	LEU
16	1U	104	GLN
16	1U	111	GLU
16	1U	112	ARG
17	1V	1	MET
17	1V	32	THR
17	1V	35	LEU
17	1V	46	VAL
17	1V	62	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	1V	72	VAL
17	1V	73	SER
17	1V	79	VAL
17	1V	82	ARG
17	1V	85	LYS
17	1V	98	GLU
17	1V	100	ARG
18	1W	17	VAL
18	1W	19	LEU
18	1W	42	ARG
18	1W	63	ASP
18	1W	65	LEU
18	1W	67	ASP
18	1W	77	ASP
18	1W	86	LEU
18	1W	100	THR
18	1W	103	ILE
18	1W	107	LEU
19	1X	23	GLU
19	1X	66	LEU
19	1X	76	ARG
20	1Y	6	HIS
20	1Y	7	VAL
20	1Y	11	ASP
20	1Y	14	LEU
20	1Y	31	LEU
20	1Y	43	ASN
20	1Y	44	ILE
20	1Y	47	LYS
20	1Y	49	VAL
20	1Y	72	VAL
20	1Y	90	LEU
21	1Z	11	GLU
21	1Z	16	SER
21	1Z	18	LEU
21	1Z	31	ARG
21	1Z	33	LEU
21	1Z	40	ASP
21	1Z	61	LEU
21	1Z	66	SER
21	1Z	76	LEU
21	1Z	86	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
21	1Z	87	ASP
21	1Z	91	LEU
21	1Z	93	ASP
21	1Z	97	GLU
21	1Z	103	ARG
21	1Z	121	HIS
21	1Z	150	LEU
21	1Z	165	VAL
21	1Z	185	GLU
21	1Z	191	VAL
21	1Z	202	GLU
21	1Z	203	GLU
22	10	39	ARG
23	11	5	CYS
23	11	21	ARG
23	11	35	THR
23	11	38	SER
23	11	59	THR
23	11	75	GLU
23	11	95	LEU
24	12	3	LEU
24	12	16	LEU
24	12	19	VAL
24	12	53	LEU
24	12	62	THR
24	12	64	LEU
25	13	3	ARG
25	13	6	VAL
25	13	8	LEU
25	13	17	LYS
25	13	23	LEU
25	13	29	ARG
25	13	44	ARG
25	13	55	ARG
25	13	56	VAL
25	13	58	VAL
26	14	5	ILE
26	14	22	ILE
26	14	23	GLU
26	14	27	THR
26	14	49	PHE
26	14	52	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
26	14	57	GLU
26	14	61	ARG
26	14	63	TYR
26	14	68	ARG
27	15	6	VAL
27	15	16	ARG
27	15	25	LEU
27	15	29	THR
27	15	57	VAL
27	15	60	VAL
28	16	4	GLU
28	16	6	ARG
28	16	9	LEU
28	16	14	THR
28	16	19	ARG
28	16	28	ARG
28	16	34	LEU
28	16	48	VAL
29	17	1	MET
29	17	4	THR
29	17	10	ARG
29	17	41	ARG
29	17	43	THR
29	17	47	ARG
29	17	48	LYS
30	18	6	THR
30	18	14	VAL
30	18	31	HIS
30	18	46	ARG
30	18	49	VAL
31	19	1	MET
31	19	3	VAL
31	19	4	ARG
31	19	26	ILE
33	1b	10	LEU
33	1b	16	HIS
33	1b	17	PHE
33	1b	19	HIS
33	1b	21	ARG
33	1b	23	ARG
33	1b	27	LYS
33	1b	45	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
33	1b	67	THR
33	1b	71	VAL
33	1b	73	THR
33	1b	74	LYS
33	1b	76	GLN
33	1b	80	ILE
33	1b	111	ARG
33	1b	128	GLU
33	1b	134	GLU
33	1b	135	GLN
33	1b	157	ARG
33	1b	172	ILE
33	1b	178	ARG
33	1b	185	ILE
33	1b	196	LEU
33	1b	215	LEU
33	1b	221	LEU
33	1b	224	GLN
33	1b	226	ARG
33	1b	230	VAL
34	1c	3	ASN
34	1c	15	THR
34	1c	29	TYR
34	1c	32	LEU
34	1c	38	ARG
34	1c	52	LEU
34	1c	64	VAL
34	1c	67	THR
34	1c	69	HIS
34	1c	85	ARG
34	1c	89	GLU
34	1c	103	VAL
34	1c	105	GLU
34	1c	115	LEU
34	1c	166	GLU
34	1c	191	THR
35	1d	3	ARG
35	1d	5	ILE
35	1d	18	LYS
35	1d	28	SER
35	1d	31	CYS
35	1d	34	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	1d	47	ARG
35	1d	58	LEU
35	1d	76	ARG
35	1d	86	LYS
35	1d	89	THR
35	1d	106	TYR
35	1d	110	PHE
35	1d	122	ARG
35	1d	127	THR
35	1d	132	ARG
35	1d	135	LEU
35	1d	141	ARG
35	1d	158	ILE
35	1d	160	GLN
35	1d	168	ARG
35	1d	173	TRP
35	1d	178	VAL
35	1d	179	GLU
35	1d	182	LYS
35	1d	188	LEU
35	1d	194	LEU
35	1d	196	LEU
36	1e	13	ILE
36	1e	16	THR
36	1e	34	VAL
36	1e	41	VAL
36	1e	69	VAL
36	1e	75	THR
36	1e	82	VAL
36	1e	91	LEU
36	1e	116	THR
37	1f	17	SER
37	1f	43	LEU
37	1f	46	ARG
37	1f	63	TYR
37	1f	69	GLU
37	1f	70	ASP
37	1f	73	ASN
38	1g	8	GLU
38	1g	21	VAL
38	1g	27	ILE
38	1g	28	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
38	1g	57	GLU
38	1g	79	ARG
38	1g	97	GLN
38	1g	98	SER
38	1g	104	LEU
38	1g	144	MET
39	1h	22	GLU
39	1h	25	ASP
39	1h	26	VAL
39	1h	39	LEU
39	1h	52	ASP
39	1h	91	ARG
39	1h	104	ARG
39	1h	107	LEU
39	1h	118	VAL
39	1h	120	THR
40	1i	19	LEU
40	1i	25	LYS
40	1i	27	THR
40	1i	31	GLN
40	1i	42	ARG
40	1i	47	LEU
40	1i	60	ASP
40	1i	64	THR
40	1i	65	VAL
40	1i	81	ILE
40	1i	96	LEU
40	1i	108	VAL
40	1i	109	VAL
40	1i	113	LYS
40	1i	114	TYR
40	1i	125	TYR
40	1i	127	LYS
41	1j	9	ARG
41	1j	13	HIS
41	1j	66	ARG
41	1j	68	HIS
41	1j	95	GLU
41	1j	100	THR
42	1k	16	SER
42	1k	18	ARG
42	1k	31	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
42	1k	96	ARG
42	1k	109	VAL
42	1k	114	VAL
43	1l	11	VAL
43	1l	18	VAL
43	1l	39	VAL
43	1l	52	LEU
43	1l	60	LEU
43	1l	67	THR
43	1l	97	ARG
43	1l	98	TYR
44	1m	56	LEU
44	1m	70	LEU
44	1m	81	LEU
44	1m	84	ILE
44	1m	102	ARG
44	1m	109	THR
44	1m	116	THR
45	1n	3	ARG
45	1n	13	THR
45	1n	18	VAL
45	1n	22	THR
45	1n	32	SER
45	1n	33	VAL
45	1n	44	LEU
46	1o	39	LEU
46	1o	68	ARG
46	1o	76	GLU
47	1p	1	MET
47	1p	2	VAL
47	1p	6	LEU
47	1p	8	ARG
47	1p	19	ILE
47	1p	20	VAL
47	1p	25	ARG
47	1p	42	ARG
47	1p	45	THR
47	1p	47	ASP
47	1p	50	LYS
47	1p	54	GLU
47	1p	60	LEU
47	1p	69	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
48	1q	6	LEU
48	1q	9	VAL
48	1q	60	ILE
48	1q	77	VAL
48	1q	81	ARG
48	1q	86	GLU
49	1r	31	LEU
49	1r	55	ARG
49	1r	65	ILE
49	1r	68	LYS
49	1r	76	LEU
50	1s	4	SER
50	1s	5	LEU
50	1s	28	LYS
50	1s	40	ILE
50	1s	71	LEU
50	1s	77	THR
50	1s	79	THR
51	1t	10	LEU
51	1t	24	LEU
51	1t	62	LEU
51	1t	71	THR
51	1t	72	LEU
51	1t	80	ARG
51	1t	81	LYS
51	1t	100	ILE
52	1u	9	ARG
52	1u	15	ARG
53	1y	2	ARG
53	1y	3	ILE
53	1y	5	PHE
53	1y	6	ARG
53	1y	15	ARG
53	1y	16	ARG
54	1z	42	SER
54	1z	58	ASN
3	2D	3	VAL
3	2D	7	LYS
3	2D	10	THR
3	2D	11	PRO
3	2D	12	SER
3	2D	13	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	2D	18	VAL
3	2D	37	LEU
3	2D	61	LEU
3	2D	94	LEU
3	2D	103	ARG
3	2D	104	TYR
3	2D	111	LEU
3	2D	127	VAL
3	2D	138	VAL
3	2D	141	VAL
3	2D	155	LEU
3	2D	165	ILE
3	2D	169	GLU
3	2D	229	VAL
3	2D	242	ARG
3	2D	253	GLN
3	2D	259	THR
4	2E	7	VAL
4	2E	9	VAL
4	2E	33	VAL
4	2E	34	VAL
4	2E	45	THR
4	2E	47	VAL
4	2E	73	GLU
4	2E	76	ARG
4	2E	93	VAL
4	2E	113	PHE
4	2E	116	VAL
4	2E	119	ARG
4	2E	144	ARG
4	2E	178	GLU
4	2E	181	LEU
4	2E	182	LEU
4	2E	184	VAL
4	2E	202	LYS
5	2F	17	ARG
5	2F	24	LEU
5	2F	27	GLU
5	2F	33	LEU
5	2F	38	ARG
5	2F	44	ARG
5	2F	53	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	2F	57	VAL
5	2F	74	ARG
5	2F	78	ILE
5	2F	82	ILE
5	2F	110	LEU
5	2F	125	LEU
5	2F	148	LEU
5	2F	157	VAL
5	2F	158	THR
5	2F	161	GLU
5	2F	162	LEU
5	2F	176	LEU
5	2F	192	LEU
5	2F	196	LEU
6	2G	28	VAL
6	2G	31	VAL
6	2G	43	LEU
6	2G	52	ILE
6	2G	53	LEU
6	2G	79	ASN
6	2G	81	LYS
6	2G	146	TYR
6	2G	150	ASP
6	2G	155	MET
6	2G	159	VAL
6	2G	165	THR
7	2H	3	ARG
7	2H	15	VAL
7	2H	52	VAL
7	2H	84	SER
7	2H	92	ILE
7	2H	105	LEU
7	2H	107	VAL
7	2H	129	THR
7	2H	136	ILE
7	2H	158	HIS
8	2I	5	LEU
8	2I	10	GLU
8	2I	12	LEU
8	2I	19	VAL
8	2I	20	ASP
8	2I	35	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	2I	38	LEU
8	2I	42	SER
8	2I	44	LEU
8	2I	57	ARG
8	2I	60	GLU
8	2I	61	ARG
8	2I	64	GLU
8	2I	75	LEU
8	2I	78	THR
8	2I	85	GLU
8	2I	109	ILE
8	2I	114	LEU
8	2I	133	HIS
8	2I	140	LEU
9	2N	1	MET
9	2N	10	GLU
9	2N	12	ARG
9	2N	33	LEU
9	2N	34	LEU
9	2N	43	THR
9	2N	55	VAL
9	2N	62	VAL
9	2N	63	THR
9	2N	65	LYS
9	2N	68	GLU
9	2N	85	ILE
9	2N	87	LEU
9	2N	93	THR
9	2N	97	ARG
9	2N	99	LEU
9	2N	138	LEU
10	2O	8	LEU
10	2O	23	ARG
10	2O	69	ILE
10	2O	96	THR
10	2O	98	VAL
10	2O	109	LYS
10	2O	117	LEU
11	2P	15	ARG
11	2P	18	ARG
11	2P	19	VAL
11	2P	32	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	2P	42	SER
11	2P	58	THR
11	2P	65	ARG
11	2P	83	VAL
11	2P	90	ARG
11	2P	125	VAL
11	2P	132	LYS
11	2P	148	LEU
12	2Q	1	MET
12	2Q	7	MET
12	2Q	8	LYS
12	2Q	17	LEU
12	2Q	18	LYS
12	2Q	35	VAL
12	2Q	55	VAL
12	2Q	75	THR
12	2Q	79	LEU
12	2Q	110	THR
12	2Q	112	GLU
13	2R	6	SER
13	2R	23	ASN
13	2R	24	GLN
13	2R	29	LEU
13	2R	33	ARG
13	2R	44	LEU
13	2R	65	LEU
13	2R	67	LEU
13	2R	86	ARG
13	2R	91	GLN
13	2R	100	LEU
13	2R	111	LEU
13	2R	114	VAL
14	2S	35	ILE
14	2S	36	TYR
14	2S	49	VAL
14	2S	50	SER
14	2S	52	SER
14	2S	59	LYS
14	2S	69	VAL
14	2S	75	GLU
14	2S	85	VAL
14	2S	110	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	2T	13	ARG
15	2T	17	THR
15	2T	40	THR
15	2T	49	VAL
15	2T	59	THR
15	2T	74	ARG
15	2T	96	ARG
15	2T	128	GLU
16	2U	5	LYS
16	2U	17	ILE
16	2U	30	LYS
16	2U	52	ARG
16	2U	74	LEU
16	2U	77	SER
16	2U	83	LEU
16	2U	95	LEU
16	2U	104	GLN
16	2U	108	GLU
16	2U	111	GLU
16	2U	112	ARG
17	2V	7	THR
17	2V	35	LEU
17	2V	38	LEU
17	2V	72	VAL
17	2V	82	ARG
17	2V	98	GLU
17	2V	100	ARG
18	2W	17	VAL
18	2W	19	LEU
18	2W	37	ARG
18	2W	39	THR
18	2W	65	LEU
18	2W	67	ASP
18	2W	77	ASP
18	2W	86	LEU
18	2W	95	ILE
18	2W	100	THR
18	2W	101	SER
18	2W	103	ILE
18	2W	107	LEU
19	2X	23	GLU
19	2X	35	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
19	2X	43	VAL
19	2X	66	LEU
19	2X	76	ARG
20	2Y	6	HIS
20	2Y	7	VAL
20	2Y	11	ASP
20	2Y	31	LEU
20	2Y	43	ASN
20	2Y	44	ILE
20	2Y	47	LYS
20	2Y	49	VAL
20	2Y	90	LEU
20	2Y	96	ILE
21	2Z	3	TYR
21	2Z	4	ARG
21	2Z	8	TYR
21	2Z	11	GLU
21	2Z	16	SER
21	2Z	19	ARG
21	2Z	31	ARG
21	2Z	33	LEU
21	2Z	37	VAL
21	2Z	40	ASP
21	2Z	71	VAL
21	2Z	76	LEU
21	2Z	86	VAL
21	2Z	91	LEU
21	2Z	103	ARG
21	2Z	121	HIS
21	2Z	150	LEU
21	2Z	165	VAL
21	2Z	180	VAL
21	2Z	185	GLU
21	2Z	191	VAL
21	2Z	202	GLU
22	20	10	THR
22	20	16	SER
22	20	39	ARG
23	21	21	ARG
23	21	38	SER
23	21	51	VAL
23	21	59	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
23	21	95	LEU
24	22	3	LEU
24	22	19	VAL
24	22	50	ILE
24	22	53	LEU
24	22	64	LEU
25	23	3	ARG
25	23	8	LEU
25	23	23	LEU
25	23	29	ARG
25	23	31	LEU
25	23	44	ARG
25	23	56	VAL
26	24	14	ILE
26	24	22	ILE
26	24	30	GLU
26	24	50	VAL
26	24	52	THR
26	24	57	GLU
26	24	61	ARG
26	24	63	TYR
26	24	68	ARG
27	25	16	ARG
27	25	25	LEU
27	25	29	THR
27	25	35	GLU
27	25	57	VAL
28	26	5	VAL
28	26	19	ARG
28	26	28	ARG
28	26	40	CYS
28	26	48	VAL
29	27	1	MET
29	27	10	ARG
29	27	24	THR
29	27	41	ARG
29	27	43	THR
29	27	47	ARG
29	27	48	LYS
30	28	6	THR
30	28	31	HIS
30	28	46	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
30	28	49	VAL
30	28	52	LYS
31	29	1	MET
31	29	9	ARG
31	29	17	ILE
31	29	26	ILE
33	2b	7	VAL
33	2b	10	LEU
33	2b	16	HIS
33	2b	17	PHE
33	2b	19	HIS
33	2b	21	ARG
33	2b	23	ARG
33	2b	24	TRP
33	2b	27	LYS
33	2b	45	GLN
33	2b	67	THR
33	2b	71	VAL
33	2b	74	LYS
33	2b	80	ILE
33	2b	87	ARG
33	2b	106	LYS
33	2b	107	THR
33	2b	111	ARG
33	2b	128	GLU
33	2b	134	GLU
33	2b	135	GLN
33	2b	157	ARG
33	2b	172	ILE
33	2b	178	ARG
33	2b	185	ILE
33	2b	196	LEU
33	2b	215	LEU
33	2b	221	LEU
33	2b	224	GLN
33	2b	226	ARG
33	2b	230	VAL
33	2b	233	SER
34	2c	3	ASN
34	2c	8	ILE
34	2c	15	THR
34	2c	32	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	2c	36	ASP
34	2c	52	LEU
34	2c	64	VAL
34	2c	82	GLU
34	2c	105	GLU
34	2c	115	LEU
34	2c	166	GLU
35	2d	3	ARG
35	2d	5	ILE
35	2d	18	LYS
35	2d	31	CYS
35	2d	34	GLU
35	2d	35	ARG
35	2d	47	ARG
35	2d	58	LEU
35	2d	76	ARG
35	2d	80	GLU
35	2d	86	LYS
35	2d	89	THR
35	2d	122	ARG
35	2d	127	THR
35	2d	135	LEU
35	2d	141	ARG
35	2d	168	ARG
35	2d	173	TRP
35	2d	179	GLU
35	2d	194	LEU
35	2d	196	LEU
35	2d	203	VAL
35	2d	208	SER
36	2e	12	LEU
36	2e	16	THR
36	2e	24	ARG
36	2e	31	LEU
36	2e	34	VAL
36	2e	41	VAL
36	2e	69	VAL
36	2e	75	THR
36	2e	82	VAL
36	2e	91	LEU
36	2e	116	THR
37	2f	43	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
37	2f	46	ARG
37	2f	63	TYR
37	2f	69	GLU
37	2f	98	LEU
38	2g	6	ARG
38	2g	8	GLU
38	2g	21	VAL
38	2g	50	ILE
38	2g	79	ARG
38	2g	97	GLN
38	2g	104	LEU
38	2g	144	MET
39	2h	25	ASP
39	2h	26	VAL
39	2h	39	LEU
39	2h	51	VAL
39	2h	54	ASP
39	2h	91	ARG
39	2h	104	ARG
39	2h	107	LEU
39	2h	120	THR
40	2i	17	VAL
40	2i	19	LEU
40	2i	25	LYS
40	2i	27	THR
40	2i	31	GLN
40	2i	47	LEU
40	2i	64	THR
40	2i	65	VAL
40	2i	96	LEU
40	2i	108	VAL
40	2i	113	LYS
40	2i	114	TYR
40	2i	125	TYR
40	2i	127	LYS
41	2j	5	ARG
41	2j	9	ARG
41	2j	66	ARG
41	2j	67	THR
41	2j	68	HIS
41	2j	89	ASP
41	2j	92	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
41	2j	95	GLU
42	2k	14	VAL
42	2k	18	ARG
42	2k	31	THR
42	2k	109	VAL
42	2k	112	THR
42	2k	114	VAL
43	2l	18	VAL
43	2l	27	LEU
43	2l	39	VAL
43	2l	41	ARG
43	2l	60	LEU
43	2l	67	THR
43	2l	97	ARG
44	2m	12	ASN
44	2m	70	LEU
44	2m	90	LEU
44	2m	102	ARG
44	2m	106	ASN
44	2m	109	THR
44	2m	111	LYS
44	2m	116	THR
45	2n	3	ARG
45	2n	6	LEU
45	2n	18	VAL
45	2n	22	THR
45	2n	32	SER
45	2n	33	VAL
45	2n	44	LEU
46	2o	3	ILE
46	2o	39	LEU
46	2o	76	GLU
47	2p	2	VAL
47	2p	6	LEU
47	2p	8	ARG
47	2p	19	ILE
47	2p	38	TYR
47	2p	42	ARG
47	2p	45	THR
47	2p	47	ASP
47	2p	50	LYS
47	2p	54	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
47	2p	60	LEU
47	2p	67	THR
47	2p	69	THR
48	2q	6	LEU
48	2q	60	ILE
48	2q	77	VAL
48	2q	81	ARG
48	2q	86	GLU
49	2r	31	LEU
49	2r	47	THR
49	2r	76	LEU
49	2r	82	THR
49	2r	85	LEU
50	2s	4	SER
50	2s	28	LYS
50	2s	67	VAL
50	2s	71	LEU
50	2s	77	THR
50	2s	79	THR
50	2s	83	HIS
51	2t	9	ASN
51	2t	10	LEU
51	2t	24	LEU
51	2t	62	LEU
51	2t	71	THR
51	2t	84	LEU
51	2t	100	ILE
52	2u	8	THR
54	2z	32	THR
54	2z	58	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (131) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	1D	96	HIS
3	1D	253	GLN
4	1E	48	GLN
4	1E	66	HIS
4	1E	143	ASN
5	1F	8	GLN
5	1F	75	HIS
5	1F	203	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	1G	41	GLN
8	1I	104	GLN
8	1I	133	HIS
10	1O	5	GLN
11	1P	27	HIS
11	1P	68	GLN
12	1Q	57	HIS
13	1R	13	HIS
14	1S	68	GLN
16	1U	104	GLN
19	1X	31	HIS
20	1Y	43	ASN
21	1Z	32	HIS
21	1Z	73	GLN
21	1Z	151	HIS
23	11	19	GLN
25	13	32	GLN
26	14	60	GLN
27	15	22	HIS
27	15	23	HIS
33	1b	40	HIS
33	1b	45	GLN
33	1b	135	GLN
33	1b	224	GLN
34	1c	6	HIS
34	1c	37	GLN
34	1c	102	ASN
34	1c	162	GLN
34	1c	176	HIS
34	1c	181	ASN
35	1d	45	GLN
35	1d	77	ASN
35	1d	119	GLN
35	1d	125	HIS
35	1d	160	GLN
35	1d	201	GLN
36	1e	73	ASN
37	1f	13	ASN
37	1f	100	ASN
38	1g	28	ASN
38	1g	86	GLN
40	1i	3	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
40	1i	34	ASN
40	1i	58	HIS
40	1i	73	GLN
40	1i	87	GLN
40	1i	117	HIS
41	1j	68	HIS
41	1j	69	ASN
43	1l	99	HIS
44	1m	92	HIS
45	1n	52	GLN
46	1o	28	GLN
48	1q	16	GLN
50	1s	83	HIS
3	2D	96	HIS
3	2D	143	HIS
3	2D	253	GLN
4	2E	48	GLN
4	2E	137	HIS
5	2F	8	GLN
5	2F	75	HIS
5	2F	203	GLN
6	2G	26	GLN
8	2I	104	GLN
8	2I	105	HIS
8	2I	133	HIS
8	2I	139	GLN
9	2N	94	HIS
9	2N	133	GLN
10	2O	89	ASN
11	2P	27	HIS
11	2P	35	HIS
13	2R	13	HIS
13	2R	23	ASN
13	2R	50	HIS
13	2R	91	GLN
14	2S	68	GLN
17	2V	80	GLN
19	2X	31	HIS
20	2Y	6	HIS
20	2Y	43	ASN
21	2Z	34	ASN
21	2Z	73	GLN

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Mol	Chain	Res	Type
21	2Z	151	HIS
22	20	50	ASN
23	21	19	GLN
25	23	32	GLN
28	26	20	ASN
33	2b	135	GLN
33	2b	212	GLN
34	2c	6	HIS
34	2c	181	ASN
35	2d	45	GLN
35	2d	77	ASN
35	2d	119	GLN
35	2d	161	ASN
37	2f	13	ASN
37	2f	32	ASN
37	2f	73	ASN
37	2f	100	ASN
38	2g	28	ASN
38	2g	86	GLN
38	2g	148	ASN
40	2i	3	GLN
40	2i	31	GLN
40	2i	34	ASN
40	2i	58	HIS
40	2i	87	GLN
40	2i	117	HIS
40	2i	124	GLN
41	2j	56	HIS
41	2j	84	GLN
42	2k	93	GLN
44	2m	77	ASN
46	2o	13	GLN
46	2o	28	GLN
46	2o	62	GLN
48	2q	16	GLN
50	2s	14	HIS
54	2z	9	GLN
54	2z	19	HIS
54	2z	90	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2901 (98%)	614 (21%)	46 (1%)
1	2A	2862/2901 (98%)	613 (21%)	51 (1%)
2	1B	119/120 (99%)	15 (12%)	0
2	2B	119/120 (99%)	19 (15%)	1 (0%)
32	1a	1494/1507 (99%)	245 (16%)	0
32	2a	1494/1507 (99%)	242 (16%)	0
All	All	8951/9056 (98%)	1748 (19%)	98 (1%)

All (1748) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	G
1	1A	12	U
1	1A	14	A
1	1A	23	G
1	1A	34	C
1	1A	39	C
1	1A	45	C
1	1A	49	A
1	1A	52	A
1	1A	61	G
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	90	U
1	1A	94	C
1	1A	95	G
1	1A	100	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	131	G
1	1A	172	C
1	1A	177	G
1	1A	181	A
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	217	G
1	1A	221	A
1	1A	222	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	224	G
1	1A	225	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	250	G
1	1A	264	C
1	1A	266	G
1	1A	271(F)	C
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(O)	C
1	1A	271(P)	C
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	272(G)	C
1	1A	275	G
1	1A	279	C
1	1A	280	C
1	1A	285	C
1	1A	311	A
1	1A	319	C
1	1A	330	A
1	1A	342	G
1	1A	352	G
1	1A	360	G
1	1A	362	U
1	1A	363	G
1	1A	370	G
1	1A	372	G
1	1A	384	U
1	1A	385	C
1	1A	386	G
1	1A	405	U
1	1A	407	G
1	1A	411	G
1	1A	412	A
1	1A	414	C
1	1A	419	C
1	1A	422	A
1	1A	423	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	428	A
1	1A	436	C
1	1A	448	U
1	1A	454	A
1	1A	456	C
1	1A	457	A
1	1A	459	U
1	1A	463	G
1	1A	464	U
1	1A	467	G
1	1A	477	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	508	G
1	1A	509	C
1	1A	510	C
1	1A	512	G
1	1A	521	G
1	1A	522	G
1	1A	528	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	562	U
1	1A	563	G
1	1A	566	U
1	1A	567	A
1	1A	573	G
1	1A	575	A
1	1A	583	G
1	1A	586	A
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(A)	U
1	1A	614(B)	G
1	1A	615	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	616	G
1	1A	619	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	647	G
1	1A	652(T)	C
1	1A	669	G
1	1A	685	A
1	1A	686	G
1	1A	699	A
1	1A	725	G
1	1A	730	C
1	1A	738	G
1	1A	739	G
1	1A	740	U
1	1A	746	A
1	1A	747	U
1	1A	751	A
1	1A	764	A
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	792	G
1	1A	796	C
1	1A	805	G
1	1A	807	U
1	1A	809	G
1	1A	811	U
1	1A	812	C
1	1A	824	A
1	1A	827	U
1	1A	828	U
1	1A	830	G
1	1A	832	G
1	1A	859	G
1	1A	873	G
1	1A	877	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	879	G
1	1A	880	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	896	A
1	1A	897	C
1	1A	910	A
1	1A	926	A
1	1A	932	G
1	1A	938	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	957	A
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	975(A)	G
1	1A	981	A
1	1A	983	A
1	1A	990	A
1	1A	995	C
1	1A	996	A
1	1A	1010	A
1	1A	1012	U
1	1A	1013	C
1	1A	1020	A
1	1A	1021	A
1	1A	1025	G
1	1A	1026	U
1	1A	1033	U
1	1A	1039	G
1	1A	1041	C
1	1A	1042	G
1	1A	1046	A
1	1A	1047	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1051	G
1	1A	1053	C
1	1A	1054	A
1	1A	1056	G
1	1A	1060	U
1	1A	1061	U
1	1A	1063	G
1	1A	1065	U
1	1A	1067	A
1	1A	1068	G
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1077	A
1	1A	1080	C
1	1A	1083	U
1	1A	1084	A
1	1A	1085	A
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1096	A
1	1A	1097	U
1	1A	1099	G
1	1A	1100	C
1	1A	1101	U
1	1A	1106	G
1	1A	1111	A
1	1A	1112	G
1	1A	1124	C
1	1A	1128	A
1	1A	1129	A
1	1A	1130	U
1	1A	1131	G
1	1A	1132	A
1	1A	1133	U
1	1A	1135	C
1	1A	1136	G
1	1A	1138	G
1	1A	1139	G
1	1A	1165	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1169	G
1	1A	1173	G
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1190	G
1	1A	1203	G
1	1A	1210	A
1	1A	1211	U
1	1A	1213	A
1	1A	1218	C
1	1A	1237	A
1	1A	1244	G
1	1A	1253	A
1	1A	1256	G
1	1A	1265	A
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1276	A
1	1A	1284	A
1	1A	1289	C
1	1A	1296	G
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1310	G
1	1A	1311	G
1	1A	1313	U
1	1A	1316	U
1	1A	1317	A
1	1A	1321	A
1	1A	1342	A
1	1A	1344	G
1	1A	1345	C
1	1A	1352	U
1	1A	1358	G
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1370	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1446	C
1	1A	1450	G
1	1A	1452	A
1	1A	1455	G
1	1A	1459	G
1	1A	1467	C
1	1A	1468	C
1	1A	1469	A
1	1A	1471	A
1	1A	1478	G
1	1A	1482	G
1	1A	1487	G
1	1A	1493	C
1	1A	1496	A
1	1A	1497	U
1	1A	1508	A
1	1A	1509	C
1	1A	1514	U
1	1A	1525	G
1	1A	1532	C
1	1A	1542	A
1	1A	1543	C
1	1A	1545	A
1	1A	1554	A
1	1A	1556	C
1	1A	1558	A
1	1A	1559	G
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1587	A
1	1A	1590	U
1	1A	1594	G
1	1A	1604	C
1	1A	1605	C
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1618	A
1	1A	1639	U
1	1A	1644	C
1	1A	1648	C
1	1A	1654	A
1	1A	1658	C
1	1A	1670	C
1	1A	1673	U
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1721	G
1	1A	1722	A
1	1A	1739	U
1	1A	1740	G
1	1A	1743	C
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1765	C
1	1A	1773	A
1	1A	1780	A
1	1A	1781	C
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1812	A
1	1A	1816	G
1	1A	1817	G
1	1A	1829	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1839	G
1	1A	1843	C
1	1A	1847	A
1	1A	1877	A
1	1A	1878	G
1	1A	1887	C
1	1A	1900	A
1	1A	1905	C
1	1A	1906	G
1	1A	1913	A
1	1A	1917	PSU
1	1A	1921	G
1	1A	1926	U
1	1A	1929	G
1	1A	1930	G
1	1A	1931	U
1	1A	1932	A
1	1A	1938	A
1	1A	1942	5MC
1	1A	1944	U
1	1A	1955	U
1	1A	1960	A
1	1A	1961	C
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1985	G
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2035	G
1	1A	2039	C
1	1A	2043	C
1	1A	2052	G
1	1A	2054	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2070	G
1	1A	2078	C
1	1A	2081	C
1	1A	2082	A
1	1A	2092	U
1	1A	2100	G
1	1A	2102	U
1	1A	2103	C
1	1A	2104	G
1	1A	2107	C
1	1A	2108	C
1	1A	2114	A
1	1A	2115	G
1	1A	2116	G
1	1A	2117	A
1	1A	2118	U
1	1A	2119	A
1	1A	2121	G
1	1A	2126	A
1	1A	2132	U
1	1A	2133	G
1	1A	2135	A
1	1A	2136	C
1	1A	2137	C
1	1A	2141	G
1	1A	2142	C
1	1A	2144	U
1	1A	2146	C
1	1A	2148	G
1	1A	2154	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2162	G
1	1A	2165	G
1	1A	2166	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2171	A
1	1A	2173	A
1	1A	2178	C
1	1A	2179	C
1	1A	2180	U
1	1A	2184	G
1	1A	2185	C
1	1A	2186	G
1	1A	2187	G
1	1A	2190	G
1	1A	2191	G
1	1A	2192	G
1	1A	2195	C
1	1A	2198	A
1	1A	2200	C
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2225	A
1	1A	2226	C
1	1A	2238	G
1	1A	2239	G
1	1A	2240	C
1	1A	2247	A
1	1A	2267	A
1	1A	2268	A
1	1A	2269	A
1	1A	2273	A
1	1A	2278	A
1	1A	2280	G
1	1A	2282	G
1	1A	2283	C
1	1A	2285	C
1	1A	2287	A
1	1A	2288	A
1	1A	2289	G
1	1A	2294	C
1	1A	2298	A
1	1A	2305	A
1	1A	2311	A
1	1A	2320	A
1	1A	2321	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2325	G
1	1A	2326	C
1	1A	2327	A
1	1A	2334	G
1	1A	2335	A
1	1A	2336	A
1	1A	2341	G
1	1A	2347	C
1	1A	2350	C
1	1A	2352	A
1	1A	2356	C
1	1A	2379	G
1	1A	2382	G
1	1A	2383	G
1	1A	2385	C
1	1A	2389	G
1	1A	2399	G
1	1A	2406	U
1	1A	2410	G
1	1A	2414	G
1	1A	2419	U
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2432	A
1	1A	2434	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2447	G
1	1A	2448	A
1	1A	2449	U
1	1A	2468	G
1	1A	2469	A
1	1A	2472	G
1	1A	2473	U
1	1A	2474	C
1	1A	2476	A
1	1A	2478	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2495	G
1	1A	2502	G
1	1A	2504	U
1	1A	2505	G
1	1A	2506	U
1	1A	2507	C
1	1A	2518	A
1	1A	2520	C
1	1A	2525	G
1	1A	2529	G
1	1A	2531	A
1	1A	2536	G
1	1A	2553	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2572	A
1	1A	2576	G
1	1A	2578	G
1	1A	2582	G
1	1A	2583	G
1	1A	2585	U
1	1A	2586	C
1	1A	2596	U
1	1A	2599	G
1	1A	2602	A
1	1A	2603	G
1	1A	2608	G
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2615	U
1	1A	2628	C
1	1A	2629	A
1	1A	2630	G
1	1A	2641	G
1	1A	2654	A
1	1A	2660	A
1	1A	2679	A
1	1A	2682	U
1	1A	2689	U
1	1A	2690	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2691	C
1	1A	2696	U
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2731	G
1	1A	2733	A
1	1A	2742	C
1	1A	2744	G
1	1A	2757	A
1	1A	2758	A
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2802	G
1	1A	2810	A
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2847	U
1	1A	2850	A
1	1A	2865	U
1	1A	2870	C
1	1A	2872	G
1	1A	2873	A
1	1A	2876	G
1	1A	2880	C
1	1A	2883	A
1	1A	2892	A
1	1A	2894	G
2	1B	2	C
2	1B	7	G
2	1B	15	A
2	1B	42	C
2	1B	45	A
2	1B	51	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	1B	56	G
2	1B	73	A
2	1B	74	U
2	1B	85	G
2	1B	89	G
2	1B	90	A
2	1B	106	G
2	1B	108	U
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	22	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	61	G
32	1a	78	G
32	1a	101	A
32	1a	115	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	151	A
32	1a	156	G
32	1a	163	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	189(F)	U
32	1a	195	A
32	1a	197	A
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	231	G
32	1a	245	C
32	1a	247	G
32	1a	251	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	253	U
32	1a	258	G
32	1a	262	A
32	1a	266	G
32	1a	267	C
32	1a	280	C
32	1a	289	G
32	1a	298	A
32	1a	321	A
32	1a	328	C
32	1a	331	G
32	1a	332	G
32	1a	348	G
32	1a	350	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	424	G
32	1a	429	U
32	1a	430	A
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	458	C
32	1a	470	C
32	1a	471	G
32	1a	485	G
32	1a	495	A
32	1a	496	A
32	1a	498	U
32	1a	500	G
32	1a	505	G
32	1a	509	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	519	C
32	1a	521	G
32	1a	531	U
32	1a	532	A
32	1a	533	A
32	1a	547	A
32	1a	558	G
32	1a	559	A
32	1a	561	U
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	630	G
32	1a	632	A
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	723	U
32	1a	731	G
32	1a	755	G
32	1a	774	G
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	829	G
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	851	G
32	1a	859	A
32	1a	870	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	960	U
32	1a	961	U
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	981	U
32	1a	982	U
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	998	G
32	1a	1001	A
32	1a	1002	G
32	1a	1003	G
32	1a	1004	A
32	1a	1006	C
32	1a	1009	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1033	G
32	1a	1036	G
32	1a	1044	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1054	C
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1070	U
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1130	A
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1147	C
32	1a	1152	A
32	1a	1159	U
32	1a	1183	A
32	1a	1184	G
32	1a	1193	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1204	A
32	1a	1208	C
32	1a	1211	U
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1224	G
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1240	U
32	1a	1241	G
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1270	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1278	U
32	1a	1280	A
32	1a	1282	C
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1317	C
32	1a	1320	C
32	1a	1322	C
32	1a	1338	G
32	1a	1340	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1370	G
32	1a	1397	C
32	1a	1400	5MC
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1445	C
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1457	G
32	1a	1469	G
32	1a	1487	G
32	1a	1492	A
32	1a	1493	A
32	1a	1497	G
32	1a	1499	A
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1507	A
32	1a	1517	G
32	1a	1529	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1530	G
32	1a	1531	A
1	2A	10	G
1	2A	15	G
1	2A	34	C
1	2A	36	G
1	2A	45	C
1	2A	61	G
1	2A	64	A
1	2A	71	A
1	2A	72	U
1	2A	74	A
1	2A	75	G
1	2A	77	C
1	2A	78	A
1	2A	90	U
1	2A	95	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	121	G
1	2A	133	C
1	2A	139(A)	G
1	2A	140	G
1	2A	154	G
1	2A	173	G
1	2A	196	A
1	2A	205	G
1	2A	208	C
1	2A	213	A
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	229	A
1	2A	230	U
1	2A	248	G
1	2A	249	C
1	2A	260	G
1	2A	264	C
1	2A	271(K)	U
1	2A	271(L)	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	271(M)	G
1	2A	271(O)	C
1	2A	271(P)	C
1	2A	272(A)	U
1	2A	272(B)	G
1	2A	272(E)	G
1	2A	272(H)	C
1	2A	275	G
1	2A	279	C
1	2A	283	A
1	2A	289	A
1	2A	294	A
1	2A	310	A
1	2A	311	A
1	2A	325	G
1	2A	330	A
1	2A	346	A
1	2A	351	G
1	2A	352	G
1	2A	353	G
1	2A	354	G
1	2A	362	U
1	2A	363	G
1	2A	363(C)	G
1	2A	363(D)	G
1	2A	370	G
1	2A	372	G
1	2A	386	G
1	2A	396	G
1	2A	399	G
1	2A	405	U
1	2A	406	G
1	2A	411	G
1	2A	412	A
1	2A	418	G
1	2A	428	A
1	2A	429	A
1	2A	435	C
1	2A	443	A
1	2A	448	U
1	2A	454	A
1	2A	455	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	457	A
1	2A	463	G
1	2A	464	U
1	2A	466	A
1	2A	471	A
1	2A	480	A
1	2A	481	G
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	510	C
1	2A	522	G
1	2A	526	A
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	549	G
1	2A	556	G
1	2A	563	G
1	2A	567	A
1	2A	573	G
1	2A	575	A
1	2A	578	A
1	2A	583	G
1	2A	593	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	609	A
1	2A	610	G
1	2A	614(A)	U
1	2A	614(B)	G
1	2A	615	G
1	2A	623	G
1	2A	627	A
1	2A	631	A
1	2A	634	C
1	2A	637	A
1	2A	644	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	645	C
1	2A	646	A
1	2A	652(T)	C
1	2A	668	G
1	2A	669	G
1	2A	686	G
1	2A	689	A
1	2A	711	G
1	2A	715	G
1	2A	717	G
1	2A	730	C
1	2A	731	C
1	2A	763	G
1	2A	764	A
1	2A	765	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	802	A
1	2A	805	G
1	2A	812	C
1	2A	820	A
1	2A	827	U
1	2A	828	U
1	2A	829	A
1	2A	846	C
1	2A	847	U
1	2A	848	G
1	2A	859	G
1	2A	866	A
1	2A	871	U
1	2A	879	G
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	896	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	907	U
1	2A	909	A
1	2A	910	A
1	2A	932	G
1	2A	938	G
1	2A	942	G
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	960	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	975(A)	G
1	2A	981	A
1	2A	983	A
1	2A	996	A
1	2A	1005	C
1	2A	1008	C
1	2A	1010	A
1	2A	1012	U
1	2A	1013	C
1	2A	1021	A
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1037	G
1	2A	1039	G
1	2A	1041	C
1	2A	1044	G
1	2A	1046	A
1	2A	1047	G
1	2A	1048	A
1	2A	1050	A
1	2A	1051	G
1	2A	1053	C
1	2A	1054	A
1	2A	1055	G
1	2A	1060	U
1	2A	1061	U
1	2A	1062	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1063	G
1	2A	1065	U
1	2A	1068	G
1	2A	1070	A
1	2A	1073	A
1	2A	1074	G
1	2A	1075	C
1	2A	1076	C
1	2A	1077	A
1	2A	1078	U
1	2A	1079	C
1	2A	1084	A
1	2A	1088	A
1	2A	1090	U
1	2A	1096	A
1	2A	1100	C
1	2A	1109	C
1	2A	1110	G
1	2A	1112	G
1	2A	1128	A
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1141	U
1	2A	1142(A)	A
1	2A	1144	G
1	2A	1148	A
1	2A	1156	A
1	2A	1169	G
1	2A	1171	G
1	2A	1173	G
1	2A	1175	U
1	2A	1176	G
1	2A	1177	A
1	2A	1178	C
1	2A	1205	U
1	2A	1206	G
1	2A	1210	A
1	2A	1211	U
1	2A	1213	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1214	A
1	2A	1220	A
1	2A	1230	C
1	2A	1237	A
1	2A	1241	A
1	2A	1245	G
1	2A	1248	G
1	2A	1253	A
1	2A	1256	G
1	2A	1262	A
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1275	A
1	2A	1277	G
1	2A	1300	U
1	2A	1301	A
1	2A	1302	A
1	2A	1313	U
1	2A	1319	G
1	2A	1321	A
1	2A	1332	G
1	2A	1338	G
1	2A	1342	A
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1363	C
1	2A	1365	A
1	2A	1370	C
1	2A	1376	C
1	2A	1378	A
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1392	A
1	2A	1397	U
1	2A	1406	U
1	2A	1416	G
1	2A	1420	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1445	A
1	2A	1445(A)	C
1	2A	1450	G
1	2A	1451	C
1	2A	1452	A
1	2A	1459	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1519	G
1	2A	1520	G
1	2A	1525	G
1	2A	1529	G
1	2A	1532	C
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1548	C
1	2A	1554	A
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1595	G
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1631	C
1	2A	1631(A)	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1635	G
1	2A	1643	G
1	2A	1648	C
1	2A	1654	A
1	2A	1661	G
1	2A	1670	C
1	2A	1674	G
1	2A	1675	C
1	2A	1676	A
1	2A	1688	U
1	2A	1695	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1705	G
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1741	A
1	2A	1750	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1772	G
1	2A	1773	A
1	2A	1774	C
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1797	C
1	2A	1798	U
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1817	G
1	2A	1826	G
1	2A	1828	G
1	2A	1829	A
1	2A	1834	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1840	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1903	G
1	2A	1906	G
1	2A	1913	A
1	2A	1927	A
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1991	U
1	2A	1992	G
1	2A	1993	U
1	2A	1994	C
1	2A	1997	G
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2043	C
1	2A	2052	G
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2063	C
1	2A	2069	G
1	2A	2079	U
1	2A	2093	G
1	2A	2097	C
1	2A	2098	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2103	C
1	2A	2104	G
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2110	G
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U
1	2A	2119	A
1	2A	2121	G
1	2A	2123	G
1	2A	2126	A
1	2A	2127	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2142	C
1	2A	2144	U
1	2A	2146	C
1	2A	2148	G
1	2A	2154	G
1	2A	2155	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2162	G
1	2A	2165	G
1	2A	2168	G
1	2A	2170	A
1	2A	2172	U
1	2A	2173	A
1	2A	2178	C
1	2A	2180	U
1	2A	2183	C
1	2A	2184	G
1	2A	2186	G
1	2A	2187	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2189	U
1	2A	2190	G
1	2A	2191	G
1	2A	2192	G
1	2A	2197	U
1	2A	2198	A
1	2A	2200	C
1	2A	2201	C
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2219	G
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2242	G
1	2A	2252	G
1	2A	2259	G
1	2A	2268	A
1	2A	2269	A
1	2A	2279	G
1	2A	2283	C
1	2A	2285	C
1	2A	2286	A
1	2A	2287	A
1	2A	2289	G
1	2A	2305	A
1	2A	2308	G
1	2A	2309	A
1	2A	2311	A
1	2A	2319	G
1	2A	2320	A
1	2A	2321	G
1	2A	2325	G
1	2A	2326	C
1	2A	2334	G
1	2A	2345	G
1	2A	2347	C
1	2A	2350	C
1	2A	2355	C
1	2A	2376	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A
1	2A	2391	G
1	2A	2400	G
1	2A	2402	C
1	2A	2406	U
1	2A	2410	G
1	2A	2414	G
1	2A	2422	A
1	2A	2425	A
1	2A	2426	A
1	2A	2428	G
1	2A	2429	G
1	2A	2430	A
1	2A	2431	U
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2449	U
1	2A	2450	A
1	2A	2452	C
1	2A	2458	G
1	2A	2468	G
1	2A	2469	A
1	2A	2474	C
1	2A	2476	A
1	2A	2480	C
1	2A	2481	G
1	2A	2487	G
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2508	G
1	2A	2510	C
1	2A	2513	G
1	2A	2517	C
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2535	G
1	2A	2536	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2574	G
1	2A	2578	G
1	2A	2585	U
1	2A	2586	C
1	2A	2596	U
1	2A	2601	C
1	2A	2602	A
1	2A	2603	G
1	2A	2608	G
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2620	C
1	2A	2629	A
1	2A	2630	G
1	2A	2634	G
1	2A	2638	G
1	2A	2641	G
1	2A	2654	A
1	2A	2663	G
1	2A	2669	G
1	2A	2677	G
1	2A	2682	U
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2748	A
1	2A	2751	G
1	2A	2752	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2757	A
1	2A	2758	A
1	2A	2765	A
1	2A	2766	G
1	2A	2775	A
1	2A	2778	A
1	2A	2780	G
1	2A	2790	A
1	2A	2791	C
1	2A	2792	G
1	2A	2793	G
1	2A	2802	G
1	2A	2808	U
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2823	A
1	2A	2833	G
1	2A	2839	G
1	2A	2849	U
1	2A	2872	G
1	2A	2874	C
1	2A	2878	U
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2895	U
2	2B	2	C
2	2B	3	C
2	2B	5	C
2	2B	7	G
2	2B	8	U
2	2B	16	G
2	2B	19	G
2	2B	34	U
2	2B	56	G
2	2B	59	A
2	2B	64	C
2	2B	72	G
2	2B	73	A
2	2B	85	G
2	2B	88	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2B	93	G
2	2B	94	C
2	2B	109	C
2	2B	110	G
32	2a	7	G
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	61	G
32	2a	78	G
32	2a	101	A
32	2a	115	G
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	151	A
32	2a	156	G
32	2a	163	C
32	2a	173	U
32	2a	174	C
32	2a	182	U
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	247	G
32	2a	251	G
32	2a	253	U
32	2a	258	G
32	2a	262	A
32	2a	266	G
32	2a	267	C
32	2a	280	C
32	2a	289	G
32	2a	298	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	348	G
32	2a	350	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	458	C
32	2a	470	C
32	2a	471	G
32	2a	485	G
32	2a	495	A
32	2a	496	A
32	2a	498	U
32	2a	500	G
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	519	C
32	2a	521	G
32	2a	527	7MG
32	2a	532	A
32	2a	533	A
32	2a	547	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	558	G
32	2a	559	A
32	2a	561	U
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	630	G
32	2a	632	A
32	2a	653	A
32	2a	661	G
32	2a	665	A
32	2a	673	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	723	U
32	2a	731	G
32	2a	755	G
32	2a	774	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	817	C
32	2a	821	G
32	2a	827	U
32	2a	828	A
32	2a	829	G
32	2a	840	C
32	2a	841	U
32	2a	848	C
32	2a	851	G
32	2a	859	A
32	2a	870	U
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	960	U
32	2a	961	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	981	U
32	2a	982	U
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	998	G
32	2a	1001	A
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A
32	2a	1006	C
32	2a	1009	G
32	2a	1020	U
32	2a	1023	G
32	2a	1024	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1033	G
32	2a	1036	G
32	2a	1044	A
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1070	U
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	1101	A
32	2a	1130	A
32	2a	1132	C
32	2a	1134	G
32	2a	1136	U
32	2a	1137	C
32	2a	1139	G
32	2a	1140	C
32	2a	1147	C
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1183	A
32	2a	1184	G
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1204	A
32	2a	1208	C
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1214	C
32	2a	1224	G
32	2a	1227	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1250	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1278	U
32	2a	1280	A
32	2a	1282	C
32	2a	1286	A
32	2a	1287	A
32	2a	1299	A
32	2a	1300	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	1302	U
32	2a	1305	G
32	2a	1317	C
32	2a	1320	C
32	2a	1322	C
32	2a	1338	G
32	2a	1340	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1370	G
32	2a	1397	C
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1445	C
32	2a	1446	U
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1457	G
32	2a	1469	G
32	2a	1487	G
32	2a	1492	A
32	2a	1493	A
32	2a	1497	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1505	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A

All (98) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	195	A
1	1A	266	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	278	A
1	1A	310	A
1	1A	503	A
1	1A	548	A
1	1A	627	A
1	1A	685	A
1	1A	764	A
1	1A	791	C
1	1A	827	U
1	1A	859	G
1	1A	945	A
1	1A	1026	U
1	1A	1045	A
1	1A	1065	U
1	1A	1067	A
1	1A	1082	U
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1210	A
1	1A	1275	A
1	1A	1419	A
1	1A	1420	U
1	1A	1442	G
1	1A	1608	A
1	1A	1609	A
1	1A	1762	A
1	1A	1800	C
1	1A	1838	C
1	1A	1929	G
1	1A	2019	A
1	1A	2225	A
1	1A	2238	G
1	1A	2422	A
1	1A	2430	A
1	1A	2439	A
1	1A	2447	G
1	1A	2448	A
1	1A	2585	U
1	1A	2598	A
1	1A	2609	U
1	1A	2689	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2756	U
1	1A	2873	A
1	2A	49	A
1	2A	195	A
1	2A	196	A
1	2A	266	G
1	2A	278	A
1	2A	310	A
1	2A	503	A
1	2A	614(A)	U
1	2A	645	C
1	2A	685	A
1	2A	774	A
1	2A	827	U
1	2A	859	G
1	2A	888	C
1	2A	945	A
1	2A	974	G
1	2A	1026	U
1	2A	1040	C
1	2A	1046	A
1	2A	1065	U
1	2A	1067	A
1	2A	1174	A
1	2A	1175	U
1	2A	1176	G
1	2A	1210	A
1	2A	1240	U
1	2A	1252	G
1	2A	1286	A
1	2A	1379	A
1	2A	1395	A
1	2A	1396	U
1	2A	1442	G
1	2A	1608	A
1	2A	1762	A
1	2A	1996	C
1	2A	2133	G
1	2A	2167	U
1	2A	2172	U
1	2A	2288	A
1	2A	2308	G

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Mol	Chain	Res	Type
1	2A	2320	A
1	2A	2335	A
1	2A	2430	A
1	2A	2439	A
1	2A	2581	G
1	2A	2585	U
1	2A	2602	A
1	2A	2689	U
1	2A	2750	A
1	2A	2756	U
1	2A	2833	G
2	2B	44	G

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

48 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
32	7MG	2a	527	32,55	22,26,27	2.53	8 (36%)	29,39,42	1.98	8 (27%)
1	5MU	1A	1915	1	19,22,23	1.14	1 (5%)	28,32,35	1.59	6 (21%)
32	7MG	1a	527	32,55	22,26,27	2.24	7 (31%)	29,39,42	1.75	8 (27%)
1	OMG	1A	2251	1	18,26,27	1.69	6 (33%)	19,38,41	1.63	5 (26%)
1	PSU	1A	2605	1	18,21,22	1.92	5 (27%)	22,30,33	1.34	3 (13%)
1	PSU	2A	1911	1	18,21,22	1.71	3 (16%)	22,30,33	1.32	3 (13%)
1	OMG	2A	2251	1	18,26,27	1.79	4 (22%)	19,38,41	2.06	7 (36%)
32	MA6	2a	1519	32	19,26,27	1.02	1 (5%)	18,38,41	4.44	3 (16%)
32	5MC	2a	967	32	18,22,23	0.76	0	26,32,35	1.35	4 (15%)
32	4OC	1a	1402	32	20,23,24	2.52	8 (40%)	26,32,35	1.15	2 (7%)
32	5MC	1a	1404	32	18,22,23	1.01	1 (5%)	26,32,35	1.43	5 (19%)
1	PSU	2A	2605	1	18,21,22	1.65	2 (11%)	22,30,33	1.80	3 (13%)
32	M2G	2a	966	32	20,27,28	3.05	6 (30%)	22,40,43	1.29	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	2MA	2A	2503	1,55	17,25,26	1.67	3 (17%)	17,37,40	0.93	1 (5%)
32	MA6	1a	1518	32	19,26,27	1.07	1 (5%)	18,38,41	5.51	3 (16%)
32	5MC	2a	1400	32	18,22,23	1.29	2 (11%)	26,32,35	1.53	5 (19%)
1	4OC	1A	1920	1	19,22,24	2.41	7 (36%)	26,31,35	1.40	4 (15%)
32	5MC	2a	1404	32	18,22,23	0.99	1 (5%)	26,32,35	1.38	3 (11%)
32	4OC	2a	1402	32	20,23,24	2.40	8 (40%)	26,32,35	1.33	2 (7%)
32	PSU	2a	516	32,55	18,21,22	1.68	4 (22%)	22,30,33	2.18	4 (18%)
32	2MG	1a	1207	32,55	18,26,27	1.97	4 (22%)	16,38,41	1.60	3 (18%)
1	PSU	2A	1917	1	18,21,22	1.15	1 (5%)	22,30,33	1.63	5 (22%)
1	5MC	1A	1962	1	18,22,23	0.94	0	26,32,35	1.69	4 (15%)
1	5MU	2A	1939	1	19,22,23	1.39	2 (10%)	28,32,35	1.65	4 (14%)
1	4OC	2A	1920	1	19,22,24	2.46	7 (36%)	26,31,35	0.82	0
43	0TD	2l	92	43	7,9,10	2.46	1 (14%)	6,11,13	3.00	3 (50%)
43	0TD	1l	92	43	7,9,10	2.42	2 (28%)	6,11,13	3.59	4 (66%)
32	UR3	2a	1498	32	19,22,23	2.02	4 (21%)	26,32,35	1.37	4 (15%)
1	5MU	1A	1939	1	19,22,23	1.45	4 (21%)	28,32,35	1.55	4 (14%)
32	M2G	1a	966	32	20,27,28	3.00	5 (25%)	22,40,43	1.50	4 (18%)
1	5MC	2A	1942	1	18,22,23	1.03	1 (5%)	26,32,35	1.20	3 (11%)
1	2MA	1A	2503	1,55	17,25,26	1.77	4 (23%)	17,37,40	1.32	3 (17%)
32	MA6	2a	1518	32	19,26,27	1.17	3 (15%)	18,38,41	4.33	4 (22%)
1	5MC	1A	1942	1	18,22,23	1.58	4 (22%)	26,32,35	1.23	3 (11%)
32	5MC	1a	1407	32	18,22,23	1.34	2 (11%)	26,32,35	1.22	4 (15%)
1	5MC	2A	1962	1,55	18,22,23	1.29	3 (16%)	26,32,35	1.26	3 (11%)
32	UR3	1a	1498	32	19,22,23	2.03	4 (21%)	26,32,35	1.36	2 (7%)
1	PSU	1A	1911	1	18,21,22	1.32	3 (16%)	22,30,33	1.72	6 (27%)
1	PSU	1A	1917	1	18,21,22	1.11	1 (5%)	22,30,33	1.63	5 (22%)
32	2MG	2a	1207	32,55	18,26,27	1.93	3 (16%)	16,38,41	1.64	3 (18%)
32	5MC	1a	1400	32	18,22,23	1.37	1 (5%)	26,32,35	1.88	6 (23%)
1	2MU	2A	2552	1,55	19,22,24	6.67	10 (52%)	26,31,36	2.67	9 (34%)
32	5MC	2a	1407	32	18,22,23	1.13	2 (11%)	26,32,35	1.26	2 (7%)
32	MA6	1a	1519	32	19,26,27	1.06	2 (10%)	18,38,41	5.04	3 (16%)
32	PSU	1a	516	32,55	18,21,22	1.28	3 (16%)	22,30,33	1.83	6 (27%)
1	5MU	2A	1915	1	19,22,23	1.49	2 (10%)	28,32,35	1.37	3 (10%)
32	5MC	1a	967	32	18,22,23	0.91	0	26,32,35	1.24	4 (15%)
1	2MU	1A	2552	1,55	19,22,24	6.54	9 (47%)	26,31,36	2.87	10 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	7MG	2a	527	32,55	-	2/7/37/38	0/3/3/3
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
32	7MG	1a	527	32,55	-	2/7/37/38	0/3/3/3
1	OMG	1A	2251	1	-	1/5/27/28	0/3/3/3
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1	-	1/5/27/28	0/3/3/3
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	5MC	1a	1404	32	-	2/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	2/7/29/30	0/3/3/3
1	2MA	2A	2503	1,55	-	2/3/25/26	0/3/3/3
32	MA6	1a	1518	32	-	3/7/29/30	0/3/3/3
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
1	4OC	1A	1920	1	-	2/9/27/30	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
32	PSU	2a	516	32,55	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32,55	-	0/5/27/28	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	1/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
43	0TD	1l	92	43	-	5/7/12/14	-
32	UR3	2a	1498	32	-	2/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,55	-	1/3/25/26	0/3/3/3
32	MA6	2a	1518	32	-	1/7/29/30	0/3/3/3
1	5MC	1A	1942	1	-	2/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	2A	1962	1,55	-	4/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	1/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	3/7/25/26	0/2/2/2
32	2MG	2a	1207	32,55	-	0/5/27/28	0/3/3/3
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
1	2MU	2A	2552	1,55	-	0/9/27/28	0/2/2/2
32	5MC	2a	1407	32	-	1/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/7/29/30	0/3/3/3
32	PSU	1a	516	32,55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	1,55	-	0/9/27/28	0/2/2/2

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2552	2MU	C4-N3	-15.00	1.11	1.38
1	2A	2552	2MU	C4-N3	-14.99	1.11	1.38
1	2A	2552	2MU	C5-C4	14.95	1.76	1.43
1	1A	2552	2MU	C5-C4	14.26	1.75	1.43
32	2a	966	M2G	C2-N3	11.34	1.44	1.30
32	1a	966	M2G	C2-N3	11.22	1.44	1.30
1	2A	2552	2MU	C6-C5	-10.48	1.10	1.35
1	1A	2552	2MU	C6-C5	-10.24	1.11	1.35
1	1A	2552	2MU	C3'-C2'	-9.39	1.32	1.52
1	2A	2552	2MU	C3'-C2'	-8.34	1.34	1.52
1	2A	2552	2MU	C6-N1	7.83	1.56	1.38
1	1A	2552	2MU	C6-N1	7.69	1.56	1.38
1	1A	2552	2MU	O4'-C4'	-6.71	1.30	1.45
1	2A	2552	2MU	O4'-C4'	-6.62	1.30	1.45
1	2A	2552	2MU	O4'-C1'	6.42	1.57	1.42
32	2a	527	7MG	C8-N9	6.23	1.49	1.46
1	2A	2552	2MU	C1'-N1	-6.18	1.29	1.47
1	2A	1920	4OC	C4-N4	5.77	1.47	1.33
32	1a	1402	4OC	C4-N4	5.70	1.47	1.35
1	1A	2552	2MU	O4'-C1'	5.62	1.55	1.42
32	1a	527	7MG	C8-N9	5.59	1.49	1.46
1	1A	2552	2MU	C1'-N1	-5.56	1.31	1.47
43	2l	92	0TD	CB-SB	-5.55	1.76	1.82
43	1l	92	0TD	CB-SB	-5.46	1.76	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	527	7MG	C5-N7	5.41	1.41	1.35
1	1A	1920	4OC	C4-N4	5.28	1.46	1.33
1	1A	2503	2MA	C2-N3	5.20	1.42	1.31
32	1a	1498	UR3	C6-C5	5.12	1.46	1.35
32	2a	1498	UR3	C6-C5	5.05	1.46	1.35
32	2a	1402	4OC	C4-N4	4.97	1.46	1.35
32	2a	516	PSU	C2-N1	4.94	1.43	1.36
32	1a	527	7MG	C5-N7	4.93	1.41	1.35
1	2A	1920	4OC	C6-C5	4.92	1.46	1.35
32	1a	1498	UR3	C2-N1	4.90	1.45	1.38
1	2A	2503	2MA	C2-N3	4.87	1.41	1.31
1	1A	1920	4OC	C2-N3	4.86	1.46	1.36
32	1a	1400	5MC	C2-N1	4.86	1.50	1.40
1	2A	2605	PSU	C2-N1	4.72	1.43	1.36
32	2a	1207	2MG	C2-N1	4.70	1.44	1.36
1	2A	1915	5MU	C2-N1	4.69	1.46	1.38
1	2A	1920	4OC	C2-N3	4.67	1.45	1.36
32	2a	527	7MG	C4-N3	4.66	1.45	1.34
32	1a	1207	2MG	C2-N2	4.64	1.43	1.33
32	2a	1498	UR3	C2-N3	4.62	1.47	1.39
32	1a	1207	2MG	C2-N1	4.51	1.43	1.36
1	2A	1939	5MU	C5M-C5	-4.43	1.39	1.50
32	1a	1402	4OC	C6-C5	4.41	1.45	1.35
1	1A	1920	4OC	C6-C5	4.41	1.45	1.35
1	1A	2605	PSU	C2-N1	4.37	1.42	1.36
32	2a	527	7MG	C2-N3	4.34	1.43	1.33
32	2a	1498	UR3	C2-N1	4.29	1.44	1.38
1	2A	1911	PSU	C2-N1	4.27	1.42	1.36
32	1a	1402	4OC	C2-N3	4.26	1.45	1.36
32	1a	966	M2G	C2-N2	4.22	1.43	1.35
32	2a	1207	2MG	C2-N2	4.20	1.42	1.33
32	2a	1402	4OC	C2-N3	4.18	1.44	1.36
32	2a	1402	4OC	C6-C5	4.16	1.44	1.35
1	2A	2251	OMG	C2-N3	4.13	1.43	1.33
32	1a	527	7MG	C4-N3	4.08	1.43	1.34
1	1A	1920	4OC	C2-N1	4.04	1.48	1.40
1	2A	2552	2MU	C3'-C4'	4.03	1.63	1.53
32	2a	966	M2G	C2-N2	3.98	1.42	1.35
1	1A	1942	5MC	C2-N1	-3.92	1.31	1.40
32	2a	1400	5MC	C2-N1	3.85	1.48	1.40
1	1A	1939	5MU	C4-C5	-3.85	1.38	1.44
1	1A	1915	5MU	C2-N1	3.82	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1402	4OC	O2-C2	-3.80	1.16	1.23
32	1a	1402	4OC	C2-N1	3.79	1.48	1.40
32	2a	1402	4OC	C4-N3	3.77	1.39	1.32
1	1A	2251	OMG	C2-N3	3.74	1.42	1.33
1	1A	1911	PSU	C2-N1	3.68	1.41	1.36
1	2A	1911	PSU	C6-N1	3.68	1.42	1.36
32	1a	1407	5MC	C2-N1	3.66	1.47	1.40
32	1a	527	7MG	C2-N3	3.66	1.42	1.33
1	1A	2503	2MA	C5-C4	-3.58	1.33	1.43
1	2A	2251	OMG	C4-N3	3.56	1.46	1.37
32	1a	1498	UR3	C2-N3	3.54	1.45	1.39
32	1a	1402	4OC	C4-N3	3.49	1.38	1.32
32	1a	1402	4OC	C5-C4	3.47	1.48	1.40
1	1A	2552	2MU	C3'-C4'	3.47	1.61	1.53
32	1a	966	M2G	C4-N3	3.44	1.45	1.37
1	2A	1911	PSU	C4-N3	3.40	1.45	1.38
1	1A	2605	PSU	C6-N1	3.40	1.41	1.36
32	1a	1207	2MG	C4-N3	3.32	1.45	1.37
32	2a	966	M2G	C4-N3	3.31	1.45	1.37
1	2A	1917	PSU	C2-N1	3.23	1.41	1.36
1	2A	1962	5MC	C4-N4	3.20	1.42	1.34
32	2a	1402	4OC	C5-C4	3.16	1.47	1.40
32	1a	1518	MA6	C5-C4	-3.16	1.32	1.40
1	2A	2251	OMG	C5-C4	-3.10	1.35	1.43
1	2A	1915	5MU	C2-N3	3.08	1.43	1.38
32	2a	1207	2MG	C4-N3	3.02	1.44	1.37
32	1a	516	PSU	C6-N1	2.99	1.41	1.36
1	1A	1917	PSU	C2-N1	2.99	1.40	1.36
1	2A	2605	PSU	C6-N1	2.98	1.41	1.36
32	1a	1402	4OC	O2-C2	-2.95	1.18	1.23
1	2A	1920	4OC	O2-C2	-2.93	1.18	1.23
32	2a	966	M2G	C2-N1	2.92	1.44	1.36
32	1a	966	M2G	C5-C4	-2.89	1.35	1.43
32	2a	527	7MG	C2-N2	2.86	1.41	1.34
32	2a	1407	5MC	C2-N1	2.85	1.46	1.40
32	2a	516	PSU	C6-N1	2.85	1.41	1.36
32	1a	527	7MG	C5-C6	2.84	1.50	1.43
32	2a	527	7MG	C5-C6	2.84	1.50	1.43
1	1A	2251	OMG	C4-N3	2.84	1.44	1.37
32	2a	516	PSU	O4'-C1'	-2.83	1.39	1.43
1	2A	1920	4OC	C5-C4	2.81	1.49	1.42
1	1A	1920	4OC	C4-N3	2.77	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1962	5MC	C2-N3	2.76	1.41	1.36
1	2A	1942	5MC	CM5-C5	-2.73	1.43	1.50
1	1A	2251	OMG	C8-N7	2.72	1.39	1.35
1	1A	2605	PSU	O4'-C1'	-2.72	1.40	1.43
32	2a	1402	4OC	CM4-N4	-2.69	1.40	1.45
32	1a	516	PSU	C2-N1	2.68	1.40	1.36
1	1A	2251	OMG	C5-C4	-2.68	1.36	1.43
32	2a	966	M2G	C5-C6	2.67	1.52	1.47
1	1A	1939	5MU	C5M-C5	-2.67	1.44	1.50
1	1A	2605	PSU	O4-C4	-2.67	1.18	1.23
1	2A	1920	4OC	C4-N3	2.66	1.39	1.34
1	1A	1939	5MU	C2-N1	-2.66	1.34	1.38
1	1A	1920	4OC	O2-C2	-2.64	1.18	1.23
32	2a	1519	MA6	C2-N3	2.64	1.36	1.32
1	2A	2503	2MA	C5-C4	-2.58	1.36	1.43
1	2A	1920	4OC	C2-N1	2.54	1.45	1.40
1	1A	1942	5MC	C4-N3	-2.53	1.30	1.34
1	2A	1939	5MU	C2-N3	2.53	1.42	1.38
32	2a	1404	5MC	CM5-C5	-2.53	1.44	1.50
32	2a	527	7MG	C2-N1	2.52	1.43	1.37
32	2a	1402	4OC	C2-N1	2.51	1.45	1.40
1	2A	2503	2MA	C4-N3	2.46	1.43	1.37
32	1a	1402	4OC	CM4-N4	-2.46	1.41	1.45
1	2A	2552	2MU	O2'-C2'	2.45	1.48	1.42
32	2a	1518	MA6	C5-C4	-2.40	1.34	1.40
32	1a	516	PSU	O4'-C1'	-2.40	1.40	1.43
32	1a	966	M2G	C2-N1	2.37	1.42	1.36
1	1A	1911	PSU	C4-C5	2.32	1.50	1.44
1	2A	1962	5MC	CM5-C5	-2.30	1.45	1.50
32	2a	966	M2G	C5-C4	-2.28	1.37	1.43
32	2a	1407	5MC	C6-C5	2.28	1.38	1.34
1	2A	2251	OMG	C6-N1	2.27	1.41	1.37
32	2a	527	7MG	C4-N9	2.26	1.40	1.37
32	1a	1519	MA6	C2-N3	2.26	1.35	1.32
1	1A	2503	2MA	C4-N3	2.25	1.42	1.37
32	2a	1518	MA6	C2-N3	2.23	1.35	1.32
32	1a	527	7MG	C2-N2	2.20	1.39	1.34
32	1a	1404	5MC	CM5-C5	-2.19	1.45	1.50
1	1A	1920	4OC	C5-C4	2.18	1.47	1.42
32	1a	1407	5MC	C6-C5	2.17	1.38	1.34
32	2a	516	PSU	C1'-C5	-2.16	1.45	1.50
1	1A	1911	PSU	C4-N3	2.16	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1498	UR3	C3U-N3	-2.16	1.43	1.47
43	1l	92	0TD	CA-N	-2.11	1.41	1.47
1	1A	2251	OMG	C2-N2	2.11	1.39	1.34
32	1a	1207	2MG	C5-C4	-2.08	1.37	1.43
32	1a	527	7MG	C2-N1	2.08	1.42	1.37
32	1a	1519	MA6	C5-C4	-2.07	1.35	1.40
1	1A	2503	2MA	C2-N1	2.07	1.43	1.36
1	1A	1942	5MC	CM5-C5	-2.06	1.45	1.50
1	1A	2605	PSU	O2-C2	2.06	1.27	1.23
32	2a	1498	UR3	C3U-N3	-2.05	1.43	1.47
1	1A	1939	5MU	C2-N3	2.04	1.41	1.38
32	2a	1518	MA6	C2-N1	2.03	1.37	1.33
1	1A	2251	OMG	O6-C6	-2.02	1.19	1.23
1	1A	1942	5MC	C6-N1	-2.02	1.34	1.38
32	2a	1400	5MC	CM5-C5	-2.01	1.45	1.50

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1518	MA6	N1-C6-N6	-20.86	95.10	117.06
32	1a	1519	MA6	N1-C6-N6	-20.17	95.83	117.06
32	2a	1519	MA6	N1-C6-N6	-17.80	98.32	117.06
32	2a	1518	MA6	N1-C6-N6	-16.69	99.49	117.06
32	2a	516	PSU	C6-C5-C4	7.96	123.77	118.20
32	1a	1518	MA6	C1'-N9-C4	-7.69	113.13	126.64
1	2A	2552	2MU	C5-C4-N3	7.25	125.69	114.84
1	1A	2552	2MU	C5-C4-N3	6.93	125.21	114.84
1	1A	2552	2MU	C4-N3-C2	-6.41	118.12	126.58
1	2A	2552	2MU	C4-N3-C2	-6.17	118.44	126.58
32	1a	1518	MA6	N3-C2-N1	-6.17	119.04	128.68
1	2A	2605	PSU	C6-C5-C4	5.98	122.38	118.20
1	2A	1939	5MU	C6-C5-C4	5.83	122.91	118.03
1	1A	2552	2MU	N3-C2-N1	5.81	122.61	114.89
32	2a	1518	MA6	C1'-N9-C4	-5.23	117.46	126.64
32	2a	527	7MG	C5-C6-N1	5.13	120.03	110.99
43	1l	92	0TD	CSB-SB-CB	5.06	111.59	102.44
43	1l	92	0TD	CB-CA-N	-5.04	98.36	109.10
32	2a	1518	MA6	N3-C2-N1	-5.02	120.83	128.68
1	1A	2552	2MU	O4-C4-C5	-4.93	116.48	125.16
1	1A	2552	2MU	O2-C2-N1	-4.79	116.42	122.79
1	1A	1962	5MC	C5-C6-N1	-4.69	118.51	123.34
32	1a	516	PSU	C6-C5-C4	4.68	121.47	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1962	5MC	C5-C4-N3	4.59	126.63	121.67
32	1a	1400	5MC	C5-C4-N3	4.55	126.59	121.67
1	2A	2552	2MU	O2-C2-N1	-4.53	116.77	122.79
43	2l	92	0TD	CSB-SB-CB	4.53	110.63	102.44
32	1a	1519	MA6	N3-C2-N1	-4.53	121.60	128.68
1	1A	1939	5MU	C6-C5-C4	4.49	121.78	118.03
1	2A	2251	OMG	O6-C6-C5	-4.46	115.66	124.37
1	1A	1917	PSU	C6-C5-C4	4.44	121.30	118.20
32	1a	1519	MA6	C1'-N9-C4	-4.42	118.88	126.64
32	1a	1400	5MC	C5-C6-N1	-4.36	118.85	123.34
1	1A	1911	PSU	C6-C5-C4	4.33	121.23	118.20
1	2A	2552	2MU	N3-C2-N1	4.33	120.64	114.89
32	2a	1400	5MC	C5-C6-N1	-4.21	119.00	123.34
32	2a	527	7MG	C2-N3-C4	4.15	119.69	112.30
32	2a	1519	MA6	N3-C2-N1	-4.14	122.21	128.68
32	2a	1400	5MC	C5-C4-N3	4.12	126.11	121.67
32	2a	1519	MA6	C1'-N9-C4	-4.10	119.43	126.64
43	1l	92	0TD	OD2-CG-CB	4.08	121.97	113.15
32	1a	1404	5MC	C5-C6-N1	-4.01	119.21	123.34
1	1A	2251	OMG	C5-C6-N1	3.96	120.95	113.95
32	1a	1498	UR3	C4-N3-C2	-3.96	120.84	124.56
1	1A	1939	5MU	C4-N3-C2	-3.96	122.23	127.35
1	1A	1942	5MC	C5-C6-N1	-3.96	119.27	123.34
1	2A	1911	PSU	C6-C5-C4	3.89	120.92	118.20
32	1a	527	7MG	C5-C6-N1	3.89	117.84	110.99
1	2A	1939	5MU	C4-N3-C2	-3.86	122.35	127.35
32	2a	1404	5MC	C5-C6-N1	-3.85	119.37	123.34
1	1A	2605	PSU	C6-C5-C4	3.84	120.88	118.20
32	2a	967	5MC	C5-C4-N3	3.83	125.80	121.67
1	2A	2251	OMG	C5-C6-N1	3.82	120.70	113.95
43	2l	92	0TD	OD2-CG-CB	3.75	121.26	113.15
1	2A	1915	5MU	C6-C5-C4	3.75	121.17	118.03
32	2a	527	7MG	C5-C4-N3	-3.69	121.09	128.13
1	2A	1917	PSU	C6-C5-C4	3.68	120.77	118.20
32	1a	527	7MG	C2-N3-C4	3.68	118.85	112.30
32	1a	527	7MG	C5-C4-N9	3.60	111.03	106.35
32	2a	1498	UR3	C1'-N1-C2	3.58	123.03	116.99
1	1A	1962	5MC	C4-N3-C2	-3.57	115.86	120.69
1	2A	2552	2MU	O4-C4-C5	-3.56	118.90	125.16
32	2a	967	5MC	C5-C6-N1	-3.56	119.68	123.34
1	1A	1915	5MU	C6-C5-C4	3.56	121.01	118.03
1	1A	1920	4OC	C1'-N1-C2	3.54	126.33	118.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2503	2MA	C5-C6-N1	3.53	120.12	114.02
32	1a	516	PSU	C6-N1-C2	-3.52	119.08	122.68
32	1a	527	7MG	C5-C4-N3	-3.49	121.47	128.13
1	2A	2251	OMG	C2-N1-C6	-3.47	118.72	125.10
32	1a	516	PSU	N1-C2-N3	3.46	119.05	115.13
32	1a	966	M2G	C2-N1-C6	-3.45	117.98	123.71
32	2a	1402	4OC	CM2-O2'-C2'	3.42	123.51	114.52
32	1a	966	M2G	C5-C6-N1	3.41	119.97	113.95
1	2A	1962	5MC	C5-C6-N1	-3.39	119.85	123.34
32	1a	967	5MC	C5-C4-N3	3.38	125.32	121.67
32	1a	1404	5MC	C5-C4-N3	3.37	125.31	121.67
32	2a	1404	5MC	C5-C4-N3	3.36	125.30	121.67
1	2A	1942	5MC	C5-C6-N1	-3.36	119.88	123.34
32	2a	1407	5MC	C5-C4-N3	3.34	125.28	121.67
32	1a	967	5MC	C5-C6-N1	-3.31	119.93	123.34
43	2l	92	0TD	CB-CA-N	-3.31	102.05	109.10
32	2a	966	M2G	C2-N1-C6	-3.18	118.42	123.71
1	2A	1917	PSU	O2-C2-N1	-3.17	119.30	122.79
32	1a	1400	5MC	CM5-C5-C6	-3.16	118.63	122.85
1	1A	1920	4OC	C1'-N1-C6	-3.15	113.97	120.84
1	2A	1915	5MU	C4-N3-C2	-3.14	123.29	127.35
1	2A	1962	5MC	C4-N3-C2	-3.13	116.45	120.69
1	2A	2552	2MU	C6-C5-C4	-3.10	115.28	119.52
32	1a	966	M2G	O6-C6-C5	-3.09	118.34	124.37
32	1a	1207	2MG	C8-N7-C5	3.07	108.83	102.99
32	2a	527	7MG	C5-C4-N9	3.05	110.31	106.35
32	1a	1400	5MC	N4-C4-N3	-3.05	112.92	118.48
32	1a	1407	5MC	C5-C6-N1	-3.03	120.22	123.34
32	1a	1207	2MG	C5-C6-N1	3.03	119.30	113.95
1	2A	1939	5MU	C5-C6-N1	-3.03	120.22	123.34
32	2a	1404	5MC	C4-N3-C2	-3.01	116.62	120.69
1	1A	1939	5MU	O4-C4-C5	-3.00	121.42	124.90
1	1A	1911	PSU	N1-C2-N3	2.96	118.49	115.13
1	1A	2251	OMG	C2-N1-C6	-2.95	119.66	125.10
32	2a	1207	2MG	C5-C6-N1	2.94	119.14	113.95
32	1a	1400	5MC	C4-N3-C2	-2.93	116.72	120.69
32	1a	1404	5MC	C4-N3-C2	-2.92	116.74	120.69
32	1a	1400	5MC	C1'-N1-C6	-2.91	116.28	121.12
32	2a	527	7MG	C4-C5-N7	2.90	109.56	105.53
1	1A	1911	PSU	O2-C2-N1	-2.87	119.63	122.79
32	1a	1498	UR3	C1'-N1-C2	2.87	121.84	116.99
32	2a	527	7MG	O6-C6-C5	-2.87	120.51	127.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1498	UR3	C4-N3-C2	-2.85	121.88	124.56
1	1A	2552	2MU	C6-C5-C4	-2.82	115.67	119.52
32	2a	1207	2MG	C8-N7-C5	2.81	108.34	102.99
32	1a	1402	4OC	O2-C2-N3	-2.81	117.76	122.33
32	2a	516	PSU	O4'-C1'-C2'	2.80	109.10	105.14
1	2A	2605	PSU	C6-N1-C2	-2.80	119.82	122.68
32	2a	967	5MC	C4-N3-C2	-2.80	116.91	120.69
32	1a	1407	5MC	C5-C4-N3	2.78	124.68	121.67
1	1A	2503	2MA	CM2-C2-N1	2.77	122.40	116.23
1	1A	1915	5MU	C4-N3-C2	-2.77	123.77	127.35
1	2A	1942	5MC	C5-C4-N3	2.76	124.65	121.67
1	1A	1911	PSU	O4-C4-N3	-2.75	114.84	120.12
32	2a	966	M2G	C5-C6-N1	2.74	118.80	113.95
32	1a	967	5MC	C4-N3-C2	-2.74	116.98	120.69
1	2A	1917	PSU	O4-C4-N3	-2.73	114.88	120.12
32	1a	527	7MG	C4-C5-N7	2.71	109.30	105.53
32	1a	1207	2MG	O3'-C3'-C2'	2.70	120.57	111.82
1	2A	2503	2MA	C5-C6-N1	2.69	118.67	114.02
32	2a	516	PSU	N1-C2-N3	2.68	118.17	115.13
32	1a	516	PSU	O4-C4-N3	-2.68	114.98	120.12
32	2a	527	7MG	C2-N1-C6	-2.67	120.24	125.10
1	2A	2605	PSU	N1-C2-N3	2.66	118.15	115.13
32	2a	1400	5MC	C4-N3-C2	-2.66	117.09	120.69
1	2A	2552	2MU	O4-C4-N3	-2.66	115.41	119.31
1	2A	2552	2MU	C4'-O4'-C1'	-2.66	103.61	109.47
32	2a	516	PSU	C6-N1-C2	-2.64	119.98	122.68
1	1A	2605	PSU	O4-C4-N3	-2.62	115.10	120.12
1	1A	1917	PSU	O2-C2-N1	-2.61	119.92	122.79
32	2a	1400	5MC	N4-C4-N3	-2.60	113.73	118.48
32	2a	1498	UR3	C3U-N3-C2	2.60	121.87	117.31
1	2A	2251	OMG	C8-N7-C5	2.57	107.89	102.99
1	1A	1917	PSU	O4-C4-N3	-2.56	115.20	120.12
1	2A	1917	PSU	N1-C2-N3	2.56	118.03	115.13
1	2A	2251	OMG	O6-C6-N1	2.53	123.63	120.65
1	1A	1911	PSU	O4-C4-C5	2.49	130.57	124.05
32	2a	1402	4OC	C6-C5-C4	2.49	120.01	116.96
1	2A	1917	PSU	C4-N3-C2	-2.49	122.75	126.34
32	1a	1404	5MC	CM5-C5-C6	-2.49	119.53	122.85
1	1A	2552	2MU	C6-N1-C2	-2.49	117.81	120.99
1	1A	2552	2MU	C1'-N1-C2	2.47	122.04	117.57
32	1a	516	PSU	O4'-C1'-C2'	2.44	108.58	105.14
1	2A	1939	5MU	C5M-C5-C6	-2.42	119.62	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1920	4OC	O2-C2-N3	-2.41	118.41	122.33
1	2A	1942	5MC	C4-N3-C2	-2.37	117.48	120.69
1	1A	2552	2MU	C4'-O4'-C1'	-2.37	104.23	109.47
32	1a	966	M2G	CM2-N2-CM1	2.37	123.11	115.77
1	2A	2251	OMG	CM2-O2'-C2'	-2.37	108.31	114.52
1	1A	1915	5MU	O4-C4-N3	-2.37	115.58	120.12
32	1a	1404	5MC	N4-C4-N3	-2.35	114.19	118.48
32	2a	1498	UR3	C6-N1-C2	-2.35	119.69	121.79
1	1A	1915	5MU	C1'-N1-C2	2.33	121.79	117.57
1	2A	1915	5MU	C1'-N1-C2	2.33	121.79	117.57
1	1A	2251	OMG	N2-C2-N1	2.32	121.65	116.71
1	1A	1920	4OC	CM2-O2'-C2'	2.30	120.57	114.52
32	2a	1407	5MC	C4-N3-C2	-2.29	117.59	120.69
32	2a	1207	2MG	CM2-N2-C2	-2.26	118.86	123.86
1	1A	1942	5MC	C4-N3-C2	-2.26	117.63	120.69
43	1l	92	0TD	OD1-CG-CB	-2.25	117.73	122.44
1	1A	2552	2MU	C3'-C2'-C1'	2.25	107.11	102.89
1	1A	1942	5MC	CM5-C5-C6	-2.24	119.85	122.85
32	2a	966	M2G	CM2-N2-CM1	2.24	122.70	115.77
32	2a	967	5MC	N4-C4-N3	-2.23	114.41	118.48
1	2A	2552	2MU	O5'-C5'-C4'	-2.21	101.47	108.99
1	1A	2251	OMG	O6-C6-C5	-2.19	120.10	124.37
1	1A	1915	5MU	O4-C4-C5	2.18	127.42	124.90
32	2a	1518	MA6	C9-N6-C6	2.18	126.10	119.51
1	1A	1911	PSU	C4-N3-C2	-2.17	123.21	126.34
1	2A	1962	5MC	CM5-C5-C6	-2.15	119.98	122.85
32	1a	527	7MG	N2-C2-N1	2.14	121.26	116.71
32	1a	1402	4OC	C6-C5-C4	2.13	119.57	116.96
1	1A	1962	5MC	C5-C4-N4	-2.13	118.29	121.48
32	1a	1407	5MC	C4-N3-C2	-2.12	117.82	120.69
32	1a	516	PSU	O4-C4-C5	2.12	129.60	124.05
1	1A	2605	PSU	O2'-C2'-C3'	-2.11	105.01	111.82
1	1A	1917	PSU	O4-C4-C5	2.10	129.56	124.05
1	1A	1915	5MU	C5M-C5-C6	-2.10	120.05	122.85
32	2a	527	7MG	N9-C4-N3	2.09	128.59	125.47
32	1a	1407	5MC	N4-C4-N3	-2.09	114.67	118.48
1	1A	1939	5MU	C5-C6-N1	-2.07	121.21	123.34
1	1A	2503	2MA	C8-N7-C5	2.06	106.91	102.99
1	2A	1911	PSU	O4-C4-N3	-2.05	116.18	120.12
1	2A	1911	PSU	O4'-C1'-C2'	2.05	108.04	105.14
32	2a	1400	5MC	CM5-C5-C6	-2.04	120.12	122.85
32	1a	967	5MC	N4-C4-N3	-2.03	114.77	118.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2251	OMG	O2'-C2'-C1'	-2.03	105.08	109.09
1	1A	1917	PSU	N1-C2-N3	2.01	117.41	115.13
1	1A	2251	OMG	C8-N7-C5	2.01	106.83	102.99
32	1a	527	7MG	O6-C6-C5	-2.01	122.60	127.54
32	1a	527	7MG	N9-C8-N7	2.01	106.25	103.38

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
1	1A	1917	PSU	C2'-C1'-C5-C4
1	1A	1917	PSU	O4'-C4'-C5'-O5'
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	SB-CB-CG-OD2
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6
1	2A	2251	OMG	C1'-C2'-O2'-CM2
32	2a	527	7MG	C3'-C4'-C5'-O5'
43	2l	92	0TD	CA-CB-SB-CSB
1	1A	1917	PSU	C3'-C4'-C5'-O5'
1	1A	1942	5MC	O4'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	2a	527	7MG	O4'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
1	1A	1942	5MC	C3'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1518	MA6	O4'-C4'-C5'-O5'
32	1a	1518	MA6	C3'-C4'-C5'-O5'
32	2a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	1404	5MC	O4'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C9
32	2a	1518	MA6	C5-C6-N6-C9
32	1a	1404	5MC	C3'-C4'-C5'-O5'
1	2A	1962	5MC	C2'-C1'-N1-C6
1	2A	2503	2MA	O4'-C4'-C5'-O5'
43	1l	92	0TD	SB-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	CA-CB-CG-OD1
1	1A	2251	OMG	C4'-C5'-O5'-P
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1498	UR3	O4'-C4'-C5'-O5'
32	1a	1498	UR3	O4'-C4'-C5'-O5'
1	1A	1920	4OC	C2'-C1'-N1-C6
32	2a	1519	MA6	C4'-C5'-O5'-P
1	2A	1962	5MC	O4'-C1'-N1-C6
1	1A	1962	5MC	O4'-C4'-C5'-O5'
1	1A	1920	4OC	C2'-C1'-N1-C2
32	1a	527	7MG	C4'-C5'-O5'-P
1	1A	2503	2MA	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	966	M2G	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
1	2A	1962	5MC	C2'-C1'-N1-C2
32	2a	1407	5MC	C2'-C1'-N1-C2
1	2A	1962	5MC	O4'-C1'-N1-C2
32	1a	527	7MG	C3'-C4'-C5'-O5'
1	2A	2503	2MA	C3'-C4'-C5'-O5'
32	2a	1498	UR3	C3'-C4'-C5'-O5'
43	2l	92	0TD	SB-CB-CG-OD1
32	2a	966	M2G	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2708 ligands modelled in this entry, 2706 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
57	SF4	2d	501	35	0,12,12	-	-	-		
57	SF4	1d	302	35	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	SF4	2d	501	35	-	-	0/6/5/5
57	SF4	1d	302	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1A	2861/2901 (98%)	-0.21	86 (3%) 50 34	9, 28, 117, 139	0
1	2A	2861/2901 (98%)	-0.19	100 (3%) 44 28	23, 45, 119, 140	0
2	1B	120/120 (100%)	-0.53	0 100 100	20, 48, 70, 100	0
2	2B	120/120 (100%)	-0.42	0 100 100	47, 69, 82, 106	0
3	1D	275/275 (100%)	-0.51	0 100 100	12, 26, 43, 74	0
3	2D	275/275 (100%)	-0.40	0 100 100	21, 38, 51, 72	0
4	1E	204/204 (100%)	-0.46	0 100 100	10, 29, 55, 71	0
4	2E	204/204 (100%)	-0.28	0 100 100	22, 44, 63, 82	0
5	1F	203/203 (100%)	-0.39	1 (0%) 91 86	8, 31, 65, 93	0
5	2F	203/203 (100%)	-0.36	0 100 100	23, 52, 77, 96	0
6	1G	181/181 (100%)	-0.32	1 (0%) 89 83	43, 68, 90, 101	0
6	2G	181/181 (100%)	0.32	14 (7%) 13 7	66, 84, 98, 106	0
7	1H	174/174 (100%)	-0.47	1 (0%) 89 83	26, 43, 62, 76	0
7	2H	174/174 (100%)	0.40	11 (6%) 20 11	52, 72, 82, 93	0
8	1I	147/147 (100%)	-0.16	0 100 100	37, 73, 88, 93	0
8	2I	147/147 (100%)	0.22	7 (4%) 30 18	47, 85, 97, 102	0
9	1N	140/140 (100%)	-0.45	0 100 100	17, 28, 59, 66	0
9	2N	140/140 (100%)	-0.16	1 (0%) 87 81	33, 49, 70, 79	0
10	1O	122/122 (100%)	-0.43	0 100 100	16, 29, 48, 57	0
10	2O	122/122 (100%)	-0.41	0 100 100	29, 41, 59, 66	0
11	1P	149/149 (100%)	-0.33	0 100 100	8, 37, 57, 83	0
11	2P	149/149 (100%)	-0.04	2 (1%) 77 65	28, 55, 78, 86	0
12	1Q	141/141 (100%)	-0.38	0 100 100	20, 32, 46, 72	0
12	2Q	141/141 (100%)	-0.35	0 100 100	35, 50, 64, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	-0.51	0 100 100	14, 23, 39, 58	0
13	2R	118/118 (100%)	-0.26	0 100 100	27, 38, 53, 66	0
14	1S	110/110 (100%)	-0.34	0 100 100	29, 45, 60, 69	0
14	2S	110/110 (100%)	0.14	4 (3%) 42 27	50, 64, 79, 82	0
15	1T	131/131 (100%)	-0.47	0 100 100	23, 35, 71, 88	0
15	2T	131/131 (100%)	-0.39	0 100 100	33, 47, 80, 92	0
16	1U	116/116 (100%)	-0.60	0 100 100	10, 19, 39, 60	0
16	2U	116/116 (100%)	-0.36	0 100 100	27, 44, 60, 66	0
17	1V	101/101 (100%)	-0.38	0 100 100	11, 29, 50, 65	0
17	2V	101/101 (100%)	-0.31	0 100 100	24, 54, 70, 75	0
18	1W	112/112 (100%)	-0.50	0 100 100	10, 19, 42, 99	0
18	2W	112/112 (100%)	-0.42	0 100 100	23, 34, 57, 97	0
19	1X	95/95 (100%)	-0.37	0 100 100	17, 27, 51, 68	0
19	2X	95/95 (100%)	-0.08	0 100 100	35, 46, 66, 76	0
20	1Y	107/107 (100%)	-0.27	1 (0%) 84 75	23, 41, 68, 78	0
20	2Y	107/107 (100%)	0.59	9 (8%) 11 6	43, 61, 78, 87	0
21	1Z	203/203 (100%)	-0.38	0 100 100	32, 57, 79, 96	0
21	2Z	203/203 (100%)	0.03	5 (2%) 57 43	53, 71, 89, 104	0
22	10	77/77 (100%)	-0.25	1 (1%) 77 65	20, 30, 52, 63	0
22	20	77/77 (100%)	0.33	8 (10%) 6 4	37, 48, 62, 70	0
23	11	97/97 (100%)	0.07	2 (2%) 63 49	17, 36, 68, 83	0
23	21	97/97 (100%)	-0.18	1 (1%) 82 72	30, 46, 74, 85	0
24	12	70/70 (100%)	-0.40	0 100 100	26, 41, 57, 87	0
24	22	70/70 (100%)	0.07	2 (2%) 51 36	47, 61, 74, 84	0
25	13	59/59 (100%)	-0.22	0 100 100	16, 26, 60, 79	0
25	23	59/59 (100%)	0.62	3 (5%) 28 16	36, 48, 71, 93	0
26	14	69/69 (100%)	-0.09	4 (5%) 23 13	62, 92, 109, 110	0
26	24	69/69 (100%)	0.38	7 (10%) 7 4	76, 100, 113, 119	0
27	15	59/59 (100%)	-0.61	0 100 100	10, 24, 45, 62	0
27	25	59/59 (100%)	-0.47	0 100 100	26, 40, 59, 82	0
28	16	53/53 (100%)	-0.44	0 100 100	28, 37, 50, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/53 (100%)	-0.11	0 100 100	41, 52, 62, 70	0
29	17	48/48 (100%)	-0.32	0 100 100	12, 17, 50, 59	0
29	27	48/48 (100%)	-0.23	1 (2%) 63 49	24, 31, 56, 72	0
30	18	64/64 (100%)	-0.41	0 100 100	15, 22, 35, 42	0
30	28	64/64 (100%)	-0.10	0 100 100	32, 39, 51, 57	0
31	19	37/37 (100%)	0.05	0 100 100	28, 36, 59, 63	0
31	29	37/37 (100%)	0.41	3 (8%) 12 6	47, 54, 70, 73	0
32	1a	1488/1507 (98%)	-0.15	33 (2%) 62 48	27, 76, 115, 143	0
32	2a	1488/1507 (98%)	-0.11	31 (2%) 63 49	33, 79, 116, 143	0
33	1b	231/231 (100%)	-0.12	7 (3%) 50 34	70, 88, 100, 113	0
33	2b	231/231 (100%)	0.03	7 (3%) 50 34	75, 91, 104, 113	0
34	1c	206/206 (100%)	-0.00	4 (1%) 66 53	72, 89, 100, 105	0
34	2c	206/206 (100%)	0.15	10 (4%) 29 17	82, 93, 104, 109	0
35	1d	208/208 (100%)	-0.18	0 100 100	57, 80, 93, 98	0
35	2d	208/208 (100%)	-0.09	1 (0%) 91 86	61, 81, 94, 103	0
36	1e	148/148 (100%)	-0.19	0 100 100	45, 69, 83, 94	0
36	2e	148/148 (100%)	-0.14	0 100 100	50, 72, 85, 100	0
37	1f	100/100 (100%)	-0.33	0 100 100	52, 71, 81, 86	0
37	2f	100/100 (100%)	-0.36	0 100 100	54, 71, 84, 88	0
38	1g	155/155 (100%)	0.09	4 (2%) 56 40	72, 84, 95, 105	0
38	2g	155/155 (100%)	0.37	15 (9%) 7 4	78, 88, 98, 106	0
39	1h	137/137 (100%)	-0.03	2 (1%) 73 61	50, 69, 79, 87	0
39	2h	137/137 (100%)	-0.07	2 (1%) 73 61	56, 73, 82, 94	0
40	1i	127/127 (100%)	0.37	8 (6%) 20 11	68, 96, 105, 108	0
40	2i	127/127 (100%)	0.79	14 (11%) 5 3	77, 99, 108, 112	0
41	1j	97/97 (100%)	0.76	12 (12%) 4 2	75, 97, 107, 113	0
41	2j	97/97 (100%)	0.88	15 (15%) 2 1	81, 100, 109, 112	0
42	1k	114/114 (100%)	-0.24	0 100 100	39, 64, 81, 90	0
42	2k	114/114 (100%)	0.03	2 (1%) 68 55	52, 71, 85, 98	0
43	1l	121/122 (99%)	-0.10	1 (0%) 86 78	42, 61, 77, 87	0
43	2l	121/122 (99%)	-0.14	0 100 100	50, 66, 79, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	116/116 (100%)	0.24	6 (5%) 27 15	71, 89, 97, 99	0
44	2m	116/116 (100%)	0.46	13 (11%) 5 3	79, 97, 104, 109	0
45	1n	60/60 (100%)	0.32	2 (3%) 46 30	70, 86, 94, 100	0
45	2n	60/60 (100%)	0.76	5 (8%) 11 6	82, 92, 100, 102	0
46	1o	88/88 (100%)	-0.07	1 (1%) 80 69	46, 66, 83, 91	0
46	2o	88/88 (100%)	-0.14	0 100 100	52, 68, 88, 93	0
47	1p	82/82 (100%)	0.37	3 (3%) 41 26	64, 78, 92, 100	0
47	2p	82/82 (100%)	0.42	3 (3%) 41 26	65, 75, 91, 101	0
48	1q	99/99 (100%)	-0.13	1 (1%) 82 72	52, 68, 79, 84	0
48	2q	99/99 (100%)	0.09	0 100 100	53, 69, 81, 86	0
49	1r	68/68 (100%)	0.16	0 100 100	53, 66, 81, 91	0
49	2r	68/68 (100%)	0.16	2 (2%) 51 36	54, 69, 86, 94	0
50	1s	83/83 (100%)	0.67	9 (10%) 5 3	78, 94, 102, 108	0
50	2s	83/83 (100%)	1.66	32 (38%) 0 0	84, 101, 111, 116	0
51	1t	96/96 (100%)	0.10	2 (2%) 63 49	65, 76, 90, 95	0
51	2t	96/96 (100%)	-0.17	1 (1%) 82 72	60, 75, 90, 93	0
52	1u	23/23 (100%)	1.21	3 (13%) 3 2	78, 84, 90, 94	0
52	2u	23/23 (100%)	1.91	14 (60%) 0 0	82, 90, 97, 99	0
53	1y	22/22 (100%)	-0.20	1 (4%) 33 21	16, 39, 78, 90	0
54	1z	97/97 (100%)	0.29	1 (1%) 82 72	52, 63, 79, 84	0
54	2z	97/97 (100%)	2.03	48 (49%) 0 0	63, 75, 85, 93	0
All	All	20796/20916 (99%)	-0.12	590 (2%) 53 37	8, 58, 104, 143	0

All (590) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1087	G	13.6
32	2a	1036	G	10.7
1	1A	1089	G	10.2
1	1A	1081	U	9.6
1	1A	1079	C	9.0
1	1A	1074	G	8.7
1	1A	1067	A	8.3
1	1A	1088	A	8.3
1	1A	1080	C	8.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2A	2139	C	8.0
1	1A	1077	A	8.0
1	1A	1064	C	7.9
1	1A	1076	C	7.8
1	2A	2802	G	7.4
1	1A	1091	G	7.3
26	14	52	THR	7.0
1	1A	1090	U	7.0
1	1A	1075	C	6.9
32	1a	1036	G	6.8
1	1A	1082	U	6.7
1	1A	1078	U	6.6
1	1A	1066	U	6.2
1	1A	1086	A	6.2
1	1A	1072	C	6.1
44	1m	115	LYS	6.1
1	1A	1063	G	6.0
41	2j	10	GLY	6.0
1	2A	2140	C	6.0
54	2z	42	SER	5.9
1	2A	2896	C	5.9
54	2z	48	PHE	5.8
1	2A	2125	G	5.8
41	1j	10	GLY	5.8
32	2a	1030(B)	C	5.8
1	2A	2147	G	5.7
1	2A	2146	C	5.6
1	1A	1092	C	5.6
1	2A	2165	G	5.5
1	2A	2124	G	5.5
1	2A	2148	G	5.5
1	1A	1093	G	5.4
40	2i	30	GLY	5.4
38	2g	156	TRP	5.4
1	1A	1083	U	5.3
32	2a	1001	A	5.3
1	1A	1103	A	5.3
50	2s	12	ASP	5.2
1	2A	2154	G	5.0
1	2A	2803	C	5.0
1	2A	2156	G	5.0
32	2a	1037	C	4.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
32	2a	1028	C	4.9
32	2a	999	C	4.9
1	1A	1068	G	4.9
32	1a	1030(B)	C	4.9
1	2A	2169	A	4.8
54	2z	10	MET	4.8
1	1A	1062	G	4.8
54	2z	38	HIS	4.8
44	2m	2	ALA	4.8
1	2A	1076	C	4.7
25	23	60	GLU	4.7
50	2s	71	LEU	4.7
1	2A	2155	G	4.7
1	2A	2110	G	4.6
32	1a	1030(C)	G	4.6
54	2z	77	LEU	4.6
32	2a	1034	G	4.6
1	2A	888	C	4.6
20	2Y	1	MET	4.6
54	2z	74	ILE	4.5
1	2A	2176	A	4.5
34	2c	158	GLY	4.5
1	2A	2162	G	4.5
32	1a	1035	A	4.5
32	2a	1020	U	4.4
54	2z	11	GLU	4.4
1	1A	2161	C	4.4
1	2A	2126	A	4.4
32	2a	1257	U	4.4
1	2A	2801(A)	A	4.3
1	1A	2140	C	4.3
1	2A	1176	G	4.3
44	2m	94	ARG	4.3
1	1A	2108	C	4.3
1	2A	2160	G	4.3
1	1A	1102	C	4.3
40	1i	8	GLY	4.2
1	1A	2116	G	4.2
6	2G	2	PRO	4.2
1	1A	1065	U	4.2
54	2z	64	SER	4.2
32	1a	1031	G	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
32	2a	78	G	4.1
50	2s	44	MET	4.1
1	1A	1057	A	4.1
1	2A	2141	G	4.1
1	2A	2132	U	4.1
1	1A	2117	A	4.1
32	2a	79	G	4.1
54	2z	41	LEU	4.1
45	2n	13	THR	4.1
1	1A	2804	C	4.1
8	2I	108	THR	4.0
1	1A	2803	C	4.0
1	2A	2123	G	4.0
32	2a	1026	G	4.0
1	1A	2173	A	4.0
32	1a	1001(A)	G	4.0
41	1j	7	LYS	4.0
54	2z	9	GLN	4.0
1	2A	2108	C	4.0
1	1A	2141	G	3.9
1	2A	2159	G	3.9
1	2A	2173	A	3.9
1	2A	2153	G	3.9
41	2j	85	LEU	3.9
40	2i	15	ALA	3.9
52	2u	10	ARG	3.9
44	2m	93	ARG	3.9
38	2g	78	ARG	3.8
1	1A	1071	G	3.8
34	2c	155	GLY	3.8
54	1z	95	ARG	3.8
44	2m	117	VAL	3.8
26	24	69	LYS	3.8
1	1A	2142	C	3.8
32	1a	1030	C	3.8
42	2k	13	GLN	3.8
1	1A	1073	A	3.8
1	1A	2147	G	3.8
1	1A	2805	G	3.8
1	2A	1175	U	3.8
54	2z	65	GLY	3.8
50	2s	82	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
54	2z	49	VAL	3.7
50	2s	47	HIS	3.7
1	2A	229	A	3.7
32	1a	1001	A	3.7
38	2g	79	ARG	3.7
32	2a	1001(A)	G	3.7
1	2A	2168	G	3.7
1	2A	2145	C	3.7
32	2a	1030(C)	G	3.7
40	1i	128	ARG	3.7
52	2u	18	TYR	3.7
1	1A	1104	C	3.7
52	1u	18	TYR	3.7
1	2A	2161	C	3.7
32	2a	998	G	3.6
40	2i	7	THR	3.6
1	2A	2174	C	3.6
32	2a	1027	C	3.6
32	1a	1037	C	3.6
1	1A	2166	G	3.6
1	2A	1087	G	3.6
40	2i	81	ILE	3.6
1	2A	2790	A	3.6
52	2u	7	ARG	3.6
1	1A	2165	G	3.6
1	1A	2139	C	3.6
41	1j	70	ARG	3.6
32	1a	1030(A)	G	3.6
1	2A	2897	U	3.5
1	2A	2106	G	3.5
34	1c	193	TYR	3.5
1	1A	2793	G	3.5
50	2s	40	ILE	3.5
1	1A	2153	G	3.5
40	1i	106	ALA	3.5
38	2g	80	VAL	3.5
50	2s	64	GLU	3.5
1	2A	2131	G	3.5
1	2A	2793	G	3.5
54	2z	45	PRO	3.5
32	2a	1531	A	3.5
54	2z	50	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
54	2z	75	ASN	3.4
32	2a	90	U	3.4
54	2z	78	ILE	3.4
32	1a	1286	A	3.4
32	1a	203	U	3.4
1	2A	2142	C	3.4
32	2a	1000	U	3.4
41	1j	35	SER	3.4
1	2A	2804	C	3.4
50	2s	66	MET	3.4
23	21	2	SER	3.4
1	2A	2157	G	3.4
38	1g	156	TRP	3.4
1	2A	2152	G	3.4
1	2A	2170	A	3.4
47	2p	59	TRP	3.4
1	2A	2127	G	3.3
1	2A	2109	U	3.3
50	2s	32	LYS	3.3
54	2z	88	LEU	3.3
21	2Z	199	LYS	3.3
1	1A	1085	A	3.3
1	1A	2801(A)	A	3.3
38	2g	154	TYR	3.3
40	1i	15	ALA	3.3
26	24	63	TYR	3.3
32	1a	1257	U	3.2
1	1A	2143	C	3.2
32	2a	1035	A	3.2
1	2A	2138	C	3.2
41	1j	34	VAL	3.2
32	1a	1034	G	3.2
41	2j	5	ARG	3.2
34	1c	204	LEU	3.2
50	2s	50	ALA	3.2
41	2j	72	VAL	3.2
54	2z	71	TYR	3.2
32	2a	1030(A)	G	3.2
1	1A	1058	G	3.2
32	2a	1033	G	3.2
20	1Y	1	MET	3.2
1	2A	2166	G	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
26	24	46	GLN	3.2
1	1A	1094	U	3.1
1	2A	2894	G	3.1
1	1A	2162	G	3.1
54	2z	39	ILE	3.1
1	2A	2175	C	3.1
32	1a	1002	G	3.1
54	2z	43	LYS	3.1
54	2z	8	LYS	3.0
54	2z	47	GLY	3.0
7	2H	13	LYS	3.0
50	2s	53	ASN	3.0
8	2I	77	LEU	3.0
52	1u	19	GLY	3.0
52	2u	22	ARG	3.0
1	1A	2132	U	3.0
1	2A	2120	G	3.0
1	1A	2127	G	3.0
1	1A	2160	G	3.0
1	2A	2807	G	3.0
54	2z	79	ASN	3.0
54	2z	72	THR	3.0
1	2A	2107	C	3.0
32	1a	204	U	3.0
7	2H	29	PRO	3.0
50	2s	57	HIS	3.0
1	1A	2167	U	3.0
20	2Y	45	VAL	3.0
33	2b	70	PHE	3.0
41	2j	47	PHE	3.0
32	1a	1003	G	2.9
29	27	48	LYS	2.9
1	1A	2123	G	2.9
1	1A	2168	G	2.9
1	2A	2121	G	2.9
26	24	45	GLY	2.9
50	2s	56	GLN	2.9
54	2z	86	ASN	2.9
1	2A	2158	A	2.9
50	2s	31	ILE	2.9
38	2g	86	GLN	2.9
1	1A	1509	C	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
54	2z	12	ILE	2.9
1	1A	888	C	2.9
1	2A	2111	C	2.9
7	2H	159	GLU	2.9
41	1j	8	LEU	2.9
44	2m	116	THR	2.9
1	1A	2112	G	2.9
1	2A	2144	U	2.8
1	2A	1084	A	2.8
32	2a	1003	G	2.8
54	2z	4	ASN	2.8
32	1a	1024	G	2.8
1	2A	652(T)	C	2.8
7	2H	95	ARG	2.8
1	2A	2164	C	2.8
26	24	64	GLY	2.8
50	1s	47	HIS	2.8
21	2Z	202	GLU	2.8
1	1A	2897	U	2.8
1	2A	11	G	2.8
32	1a	1026	G	2.8
26	14	59	PHE	2.8
54	2z	40	ILE	2.8
44	2m	69	GLU	2.8
54	2z	66	LYS	2.8
6	2G	26	GLN	2.8
50	2s	81	ARG	2.8
1	2A	1086	A	2.8
32	1a	1030(D)	A	2.8
22	10	8	GLY	2.7
54	2z	20	VAL	2.7
32	2a	1005	A	2.7
52	2u	9	ARG	2.7
1	2A	2172	U	2.7
1	1A	2152	G	2.7
1	2A	2792	G	2.7
7	2H	103	LEU	2.7
41	2j	98	ILE	2.7
1	1A	2146	C	2.7
1	2A	1067	A	2.7
33	1b	136	VAL	2.7
50	2s	61	TYR	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
54	2z	6	THR	2.7
35	2d	157	LEU	2.7
34	2c	162	GLN	2.7
50	1s	38	SER	2.7
51	1t	55	ILE	2.7
1	2A	652(S)	C	2.7
38	2g	16	LEU	2.7
26	24	68	ARG	2.7
31	29	37	GLY	2.7
41	2j	62	HIS	2.7
54	2z	67	HIS	2.7
44	2m	90	LEU	2.7
22	20	70	GLN	2.7
54	2z	73	ALA	2.7
33	1b	126	GLU	2.6
50	1s	40	ILE	2.6
32	1a	1006	C	2.6
38	2g	8	GLU	2.6
51	1t	9	ASN	2.6
54	2z	87	LYS	2.6
6	2G	157	ILE	2.6
8	2I	68	LEU	2.6
50	1s	66	MET	2.6
1	1A	2125	G	2.6
22	20	8	GLY	2.6
45	2n	12	ARG	2.6
40	1i	7	THR	2.6
25	23	26	LEU	2.6
32	2a	1004	A	2.6
1	2A	1064	C	2.6
32	2a	1007	C	2.6
45	1n	16	PHE	2.6
1	1A	2144	U	2.6
50	2s	75	ALA	2.6
1	2A	2105	C	2.6
1	2A	2137	C	2.6
8	2I	111	PRO	2.6
50	2s	48	THR	2.6
22	20	76	GLY	2.6
50	2s	69	HIS	2.6
1	2A	1083	U	2.6
50	2s	49	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	2A	652(F)	G	2.6
1	1A	2896	C	2.6
1	1A	2159	G	2.6
41	2j	65	LEU	2.6
26	24	52	THR	2.6
21	2Z	198	LYS	2.5
1	1A	2107	C	2.5
38	2g	82	GLY	2.5
1	1A	2172	U	2.5
54	2z	5	ILE	2.5
1	2A	2163	C	2.5
32	1a	1044	A	2.5
25	23	6	VAL	2.5
39	2h	131	GLY	2.5
34	1c	196	LEU	2.5
50	2s	3	ARG	2.5
32	1a	202	U	2.5
38	2g	9	VAL	2.5
40	1i	30	GLY	2.5
47	1p	4	ILE	2.5
1	2A	1082	U	2.5
33	2b	132	LYS	2.5
50	1s	71	LEU	2.5
41	1j	75	ILE	2.5
1	1A	2109	U	2.5
34	1c	206	GLU	2.5
53	1y	17	PRO	2.5
50	2s	79	THR	2.5
38	1g	16	LEU	2.5
50	2s	11	VAL	2.5
1	2A	1509	C	2.5
41	1j	71	LEU	2.5
50	1s	61	TYR	2.5
41	2j	6	ILE	2.5
44	2m	110	ARG	2.5
45	2n	8	GLU	2.5
32	2a	1030	C	2.4
32	2a	1137	C	2.4
40	1i	47	LEU	2.4
39	1h	62	TYR	2.4
26	14	51	ASP	2.4
7	2H	41	MET	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
23	11	2	SER	2.4
1	2A	1044	G	2.4
8	2I	3	VAL	2.4
26	14	64	GLY	2.4
32	1a	1033	G	2.4
6	1G	80	PHE	2.4
20	2Y	50	ARG	2.4
40	2i	29	ASN	2.4
38	2g	6	ARG	2.4
34	2c	196	LEU	2.4
38	2g	76	ARG	2.4
34	2c	157	ILE	2.4
32	1a	1028	C	2.4
7	2H	48	GLY	2.4
33	1b	122	PHE	2.4
45	2n	7	ILE	2.4
50	1s	74	PHE	2.4
32	2a	1286	A	2.4
34	2c	206	GLU	2.4
6	2G	41	GLN	2.4
22	20	50	ASN	2.4
54	2z	14	PRO	2.4
39	1h	58	TYR	2.4
44	1m	117	VAL	2.4
20	2Y	106	LEU	2.4
20	2Y	5	MET	2.4
40	2i	65	VAL	2.4
41	2j	63	PHE	2.4
54	2z	51	ASP	2.4
1	1A	1175	U	2.4
41	2j	34	VAL	2.4
1	2A	2185	C	2.4
50	2s	6	LYS	2.4
1	1A	2794	C	2.4
45	2n	39	LEU	2.4
46	1o	89	GLY	2.3
24	22	8	LYS	2.3
1	2A	2133	G	2.3
52	2u	13	ILE	2.3
1	2A	2143	C	2.3
32	1a	1000	U	2.3
50	1s	49	ILE	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
33	2b	122	PHE	2.3
54	2z	58	ASN	2.3
1	1A	2174	C	2.3
32	1a	1027	C	2.3
1	1A	2169	A	2.3
6	2G	62	LEU	2.3
52	2u	6	ARG	2.3
1	1A	652(S)	C	2.3
1	2A	2116	G	2.3
41	2j	97	GLU	2.3
33	2b	137	ARG	2.3
50	2s	74	PHE	2.3
22	20	74	ARG	2.3
50	2s	63	THR	2.3
52	2u	21	TYR	2.3
44	1m	97	PRO	2.3
52	2u	19	GLY	2.3
38	2g	84	ASN	2.3
40	1i	46	ALA	2.3
44	2m	83	ASP	2.3
11	2P	149	GLU	2.3
54	2z	37	PRO	2.3
6	2G	82	LEU	2.3
7	2H	43	VAL	2.3
21	2Z	200	GLY	2.3
33	1b	130	ARG	2.3
44	1m	114	ARG	2.3
32	1a	1004	A	2.3
24	22	1	MET	2.3
44	1m	96	LEU	2.3
6	2G	39	ILE	2.3
20	2Y	55	TYR	2.3
32	2a	1029	C	2.3
41	2j	27	ALA	2.3
9	2N	140	VAL	2.3
54	2z	52	ALA	2.3
1	1A	2124	G	2.2
6	2G	142	PRO	2.2
41	1j	98	ILE	2.2
40	2i	110	GLU	2.2
7	2H	105	LEU	2.2
1	2A	1058	G	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2A	2805	G	2.2
45	1n	17	LYS	2.2
6	2G	87	PRO	2.2
50	1s	56	GLN	2.2
1	2A	2895	U	2.2
38	1g	85	TYR	2.2
44	2m	82	MET	2.2
41	1j	69	ASN	2.2
52	1u	22	ARG	2.2
14	2S	52	SER	2.2
41	2j	99	LYS	2.2
50	2s	13	ASP	2.2
50	2s	80	TYR	2.2
51	2t	9	ASN	2.2
1	1A	2119	A	2.2
1	2A	1088	A	2.2
8	2I	4	ILE	2.2
31	29	24	TYR	2.2
43	1l	64	TYR	2.2
22	20	69	PHE	2.2
1	2A	2119	A	2.2
54	2z	89	GLN	2.2
33	1b	214	ILE	2.2
1	1A	2113	U	2.2
23	1l	23	LYS	2.2
32	1a	1532	U	2.2
49	2r	23	LYS	2.2
50	2s	4	SER	2.2
54	2z	63	ALA	2.2
1	1A	2126	A	2.2
41	1j	73	ASP	2.2
21	2Z	191	VAL	2.2
54	2z	70	MET	2.2
54	2z	24	LEU	2.2
33	2b	131	PRO	2.2
7	2H	47	GLU	2.2
6	2G	136	ARG	2.2
1	2A	2136	C	2.1
54	2z	46	GLN	2.1
42	2k	80	VAL	2.1
22	20	75	LEU	2.1
8	2I	100	ALA	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2A	1104	C	2.1
40	2i	70	LYS	2.1
54	2z	91	LYS	2.1
38	2g	81	GLY	2.1
54	2z	92	GLY	2.1
14	2S	58	LEU	2.1
20	2Y	60	PHE	2.1
6	2G	75	LYS	2.1
38	2g	32	ARG	2.1
1	1A	2164	C	2.1
52	2u	11	GLY	2.1
48	1q	36	ILE	2.1
1	1A	2894	G	2.1
1	2A	2117	A	2.1
1	2A	2151	G	2.1
1	2A	2893	G	2.1
1	2A	2179	C	2.1
34	2c	160	ALA	2.1
41	2j	84	GLN	2.1
1	2A	2118	U	2.1
50	2s	83	HIS	2.1
50	2s	30	LEU	2.1
40	2i	18	PHE	2.1
14	2S	55	ALA	2.1
38	1g	78	ARG	2.1
49	2r	29	PHE	2.1
34	2c	202	ILE	2.1
50	2s	45	VAL	2.1
52	2u	14	TRP	2.1
52	2u	24	ARG	2.1
54	2z	17	ARG	2.1
32	1a	1005	A	2.1
40	2i	36	TYR	2.1
34	2c	39	ILE	2.1
33	1b	135	GLN	2.1
22	20	77	ARG	2.1
44	1m	32	GLU	2.1
47	1p	50	LYS	2.1
1	2A	2791	C	2.1
32	2a	1006	C	2.1
40	2i	14	VAL	2.1
6	2G	88	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
31	29	12	ASP	2.1
39	2h	130	GLY	2.1
44	2m	111	LYS	2.1
52	2u	12	LYS	2.1
6	2G	152	LEU	2.1
33	1b	187	LEU	2.1
1	2A	2794	C	2.1
5	1F	15	SER	2.1
32	1a	1032	G	2.0
20	2Y	65	ALA	2.0
47	1p	7	ALA	2.0
47	2p	36	ILE	2.0
33	2b	133	LYS	2.0
11	2P	94	GLU	2.0
40	2i	62	TYR	2.0
1	2A	2171	A	2.0
1	2A	2892	A	2.0
7	2H	82	GLY	2.0
34	2c	197	GLY	2.0
40	2i	8	GLY	2.0
52	2u	17	THR	2.0
7	1H	2	SER	2.0
14	2S	53	SER	2.0
44	2m	87	TYR	2.0
6	2G	135	LEU	2.0
40	2i	47	LEU	2.0
47	2p	19	ILE	2.0
1	2A	2167	U	2.0
44	2m	92	HIS	2.0
20	2Y	75	ILE	2.0
1	1A	2131	G	2.0
41	1j	37	PRO	2.0
32	1a	1531	A	2.0
32	1a	1533	C	2.0
33	2b	136	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	5MU	1A	1915	21/22	0.93	0.25	81,89,96,98	0
1	PSU	1A	1917	20/21	0.93	0.16	61,75,81,85	0
32	PSU	1a	516	20/21	0.93	0.17	69,78,82,84	0
32	PSU	2a	516	20/21	0.93	0.19	72,81,90,91	0
32	7MG	2a	527	24/25	0.93	0.23	61,66,74,77	0
32	M2G	2a	966	25/26	0.93	0.18	65,73,81,86	0
1	PSU	2A	1917	20/21	0.94	0.13	76,81,94,98	0
32	5MC	1a	1407	21/22	0.94	0.18	38,55,60,63	0
1	PSU	2A	1911	20/21	0.94	0.10	65,72,79,80	0
1	5MU	2A	1915	21/22	0.94	0.18	86,95,109,116	0
1	4OC	2A	1920	21/23	0.95	0.15	55,67,70,73	0
32	2MG	1a	1207	24/25	0.95	0.16	82,91,97,98	0
32	4OC	1a	1402	22/23	0.95	0.20	51,55,61,63	0
1	PSU	1A	1911	20/21	0.95	0.13	64,69,74,74	0
32	5MC	2a	967	21/22	0.95	0.15	65,74,83,89	0
32	2MG	2a	1207	24/25	0.95	0.22	91,98,105,108	0
32	4OC	2a	1402	22/23	0.95	0.17	56,59,64,70	0
32	7MG	1a	527	24/25	0.96	0.19	52,56,64,67	0
1	5MC	2A	1942	21/22	0.96	0.19	37,44,48,50	0
32	M2G	1a	966	25/26	0.96	0.16	56,64,75,80	0
32	5MC	2a	1400	21/22	0.96	0.21	64,68,73,77	0
32	5MC	1a	967	21/22	0.96	0.18	61,69,81,82	0
32	5MC	2a	1404	21/22	0.96	0.15	47,54,61,64	0
32	5MC	2a	1407	21/22	0.96	0.14	50,59,65,66	0
32	UR3	2a	1498	21/22	0.96	0.17	47,52,58,61	0
32	MA6	2a	1518	24/25	0.96	0.18	43,53,58,61	0
1	PSU	2A	2605	20/21	0.97	0.17	21,28,33,36	0
32	UR3	1a	1498	21/22	0.97	0.19	39,50,58,61	0
43	0TD	1l	92	10/11	0.97	0.23	64,66,69,72	0
1	5MU	1A	1939	21/22	0.97	0.19	14,22,25,27	0
32	5MC	1a	1400	21/22	0.97	0.17	51,55,58,60	0
1	PSU	1A	2605	20/21	0.97	0.18	11,17,22,26	0
32	5MC	1a	1404	21/22	0.97	0.13	42,50,53,57	0
1	5MU	2A	1939	21/22	0.97	0.18	26,31,36,40	0
1	4OC	1A	1920	21/23	0.97	0.17	47,60,68,69	0
1	5MC	2A	1962	21/22	0.97	0.12	32,41,48,55	0
1	OMG	2A	2251	24/25	0.97	0.17	29,34,37,43	0
1	2MA	2A	2503	23/24	0.97	0.18	19,23,26,34	0
32	MA6	2a	1519	24/25	0.97	0.24	44,51,54,55	0
43	0TD	2l	92	10/11	0.97	0.20	64,71,79,83	0
32	MA6	1a	1518	24/25	0.98	0.18	36,42,45,48	0
32	MA6	1a	1519	24/25	0.98	0.19	34,40,44,49	0
1	2MA	1A	2503	23/24	0.98	0.18	7,11,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	5MC	1A	1942	21/22	0.98	0.17	19,27,30,36	0
1	5MC	1A	1962	21/22	0.98	0.15	25,29,32,41	0
1	OMG	1A	2251	24/25	0.98	0.16	17,21,27,28	0
1	2MU	2A	2552	21/23	0.98	0.17	24,29,32,34	0
1	2MU	1A	2552	21/23	0.99	0.20	15,19,22,25	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2B	3016	1/1	-0.10	0.96	85,85,85,85	0
55	MG	2H	8001	1/1	-0.01	0.75	93,93,93,93	0
55	MG	2A	3911	1/1	0.09	0.87	53,53,53,53	0
55	MG	2A	3764	1/1	0.17	0.83	70,70,70,70	0
55	MG	2a	1613	1/1	0.27	0.28	72,72,72,72	0
55	MG	2A	3260	1/1	0.29	0.19	94,94,94,94	0
55	MG	2a	1754	1/1	0.30	0.27	104,104,104,104	0
55	MG	2a	1672	1/1	0.36	0.60	64,64,64,64	0
55	MG	2B	3014	1/1	0.37	0.56	76,76,76,76	0
55	MG	2i	3001	1/1	0.37	0.45	73,73,73,73	0
55	MG	1A	3256	1/1	0.38	0.29	68,68,68,68	0
55	MG	1A	3170	1/1	0.39	0.37	62,62,62,62	0
55	MG	2a	1838	1/1	0.40	0.19	111,111,111,111	0
55	MG	1a	1676	1/1	0.41	0.43	46,46,46,46	0
55	MG	1a	1835	1/1	0.43	0.75	81,81,81,81	0
55	MG	2G	3001	1/1	0.43	0.30	92,92,92,92	0
55	MG	2a	1779	1/1	0.45	0.31	92,92,92,92	0
55	MG	2A	3279	1/1	0.45	0.64	83,83,83,83	0
55	MG	1A	3048	1/1	0.45	0.66	43,43,43,43	0
55	MG	2g	3001	1/1	0.46	0.32	64,64,64,64	0
55	MG	1A	3085	1/1	0.46	0.65	32,32,32,32	0
55	MG	2A	3694	1/1	0.48	1.05	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3591	1/1	0.49	0.54	50,50,50,50	0
55	MG	2B	3006	1/1	0.51	0.21	64,64,64,64	0
55	MG	2A	3800	1/1	0.51	0.44	73,73,73,73	0
55	MG	1a	1659	1/1	0.51	0.23	70,70,70,70	0
55	MG	2a	1724	1/1	0.52	0.28	96,96,96,96	0
55	MG	2A	3051	1/1	0.52	0.57	51,51,51,51	0
55	MG	2A	3419	1/1	0.52	0.63	60,60,60,60	0
55	MG	1B	217	1/1	0.53	0.55	57,57,57,57	0
55	MG	2a	1643	1/1	0.55	0.70	86,86,86,86	0
55	MG	2A	3784	1/1	0.55	0.79	86,86,86,86	0
55	MG	2A	3187	1/1	0.55	0.51	63,63,63,63	0
55	MG	2B	3026	1/1	0.55	0.94	83,83,83,83	0
55	MG	1A	3553	1/1	0.56	1.03	37,37,37,37	0
55	MG	1a	1661	1/1	0.56	0.81	67,67,67,67	0
55	MG	2a	1830	1/1	0.57	0.30	119,119,119,119	0
55	MG	1a	1753	1/1	0.57	0.20	81,81,81,81	0
55	MG	2A	3623	1/1	0.58	0.27	54,54,54,54	0
55	MG	1a	1644	1/1	0.58	0.42	70,70,70,70	0
55	MG	2a	1671	1/1	0.59	0.35	49,49,49,49	0
55	MG	1A	3528	1/1	0.59	1.34	31,31,31,31	0
55	MG	2a	1834	1/1	0.59	0.59	76,76,76,76	0
55	MG	1a	1763	1/1	0.60	0.14	91,91,91,91	0
55	MG	2A	3939	1/1	0.60	1.17	53,53,53,53	0
55	MG	1a	1680	1/1	0.62	0.41	65,65,65,65	0
55	MG	1a	1770	1/1	0.62	0.49	53,53,53,53	0
55	MG	2a	1783	1/1	0.62	0.12	90,90,90,90	0
55	MG	2a	1663	1/1	0.62	0.53	86,86,86,86	0
55	MG	2a	1665	1/1	0.62	0.68	48,48,48,48	0
55	MG	2A	3781	1/1	0.62	0.50	53,53,53,53	0
55	MG	2A	3644	1/1	0.62	0.62	48,48,48,48	0
55	MG	2B	3008	1/1	0.62	0.60	69,69,69,69	0
55	MG	2a	1678	1/1	0.63	0.25	60,60,60,60	0
55	MG	2a	1619	1/1	0.64	0.66	95,95,95,95	0
55	MG	2A	3116	1/1	0.64	1.08	45,45,45,45	0
55	MG	2A	3326	1/1	0.64	0.26	54,54,54,54	0
55	MG	2A	3176	1/1	0.64	0.54	81,81,81,81	0
55	MG	1X	102	1/1	0.65	0.58	49,49,49,49	0
55	MG	2A	3753	1/1	0.65	0.83	41,41,41,41	0
55	MG	2A	3888	1/1	0.65	0.36	63,63,63,63	0
55	MG	2A	3109	1/1	0.65	0.46	43,43,43,43	0
55	MG	2B	3023	1/1	0.65	0.33	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	2a	1748	1/1	0.65	0.28	71,71,71,71	0
55	MG	1A	3253	1/1	0.65	1.00	59,59,59,59	0
55	MG	2B	3025	1/1	0.66	0.38	63,63,63,63	0
55	MG	2A	3046	1/1	0.66	0.29	50,50,50,50	0
55	MG	2D	308	1/1	0.66	0.51	64,64,64,64	0
55	MG	2D	314	1/1	0.66	0.36	50,50,50,50	0
55	MG	2D	315	1/1	0.66	0.16	60,60,60,60	0
55	MG	1a	1614	1/1	0.66	0.36	75,75,75,75	0
55	MG	1A	3061	1/1	0.66	0.18	34,34,34,34	0
55	MG	20	102	1/1	0.66	0.20	66,66,66,66	0
55	MG	20	104	1/1	0.66	0.32	62,62,62,62	0
55	MG	2A	3915	1/1	0.67	0.78	70,70,70,70	0
55	MG	2A	3727	1/1	0.67	0.43	67,67,67,67	0
55	MG	2A	3559	1/1	0.67	0.98	63,63,63,63	0
55	MG	2a	1624	1/1	0.67	0.46	62,62,62,62	0
55	MG	2A	3164	1/1	0.68	0.46	44,44,44,44	0
55	MG	2a	1796	1/1	0.68	0.80	95,95,95,95	0
55	MG	2a	1828	1/1	0.68	0.44	90,90,90,90	0
55	MG	1a	1828	1/1	0.68	0.39	74,74,74,74	0
55	MG	2A	3945	1/1	0.68	0.61	81,81,81,81	0
55	MG	2A	3073	1/1	0.68	0.27	41,41,41,41	0
55	MG	1A	3650	1/1	0.68	0.52	76,76,76,76	0
55	MG	1A	3255	1/1	0.68	0.15	57,57,57,57	0
55	MG	2Y	201	1/1	0.69	1.18	61,61,61,61	0
55	MG	1a	1684	1/1	0.69	0.72	44,44,44,44	0
55	MG	2a	1820	1/1	0.69	0.27	51,51,51,51	0
55	MG	1A	3717	1/1	0.69	0.60	29,29,29,29	0
55	MG	1a	1666	1/1	0.69	0.85	42,42,42,42	0
55	MG	2B	3009	1/1	0.69	1.03	72,72,72,72	0
55	MG	1d	301	1/1	0.69	0.11	110,110,110,110	0
55	MG	2A	3923	1/1	0.69	0.36	83,83,83,83	0
55	MG	2A	3521	1/1	0.69	0.34	48,48,48,48	0
55	MG	2z	101	1/1	0.69	1.02	111,111,111,111	0
56	ZN	24	501	1/1	0.69	0.08	150,150,150,150	0
55	MG	2A	3194	1/1	0.70	0.65	40,40,40,40	0
55	MG	1n	502	1/1	0.70	0.24	74,74,74,74	0
55	MG	1a	1771	1/1	0.70	0.15	92,92,92,92	0
55	MG	2A	3720	1/1	0.70	0.46	60,60,60,60	0
55	MG	2A	3885	1/1	0.70	0.17	67,67,67,67	0
55	MG	2a	1747	1/1	0.70	0.23	106,106,106,106	0
55	MG	2A	3580	1/1	0.70	0.31	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	2A	3735	1/1	0.70	0.10	103,103,103,103	0
55	MG	2a	1651	1/1	0.70	0.45	60,60,60,60	0
55	MG	1a	1759	1/1	0.70	0.16	94,94,94,94	0
55	MG	2B	3017	1/1	0.71	0.34	68,68,68,68	0
55	MG	2a	1666	1/1	0.71	0.32	68,68,68,68	0
55	MG	1A	3685	1/1	0.71	0.26	43,43,43,43	0
55	MG	2d	502	1/1	0.71	0.29	48,48,48,48	0
55	MG	2A	3917	1/1	0.71	0.33	71,71,71,71	0
55	MG	2A	3202	1/1	0.71	0.67	61,61,61,61	0
55	MG	1A	3480	1/1	0.71	0.49	45,45,45,45	0
55	MG	1A	3957	1/1	0.71	0.41	78,78,78,78	0
55	MG	2a	1615	1/1	0.72	0.38	80,80,80,80	0
55	MG	1a	1672	1/1	0.72	0.37	70,70,70,70	0
55	MG	1A	3912	1/1	0.72	0.45	35,35,35,35	0
55	MG	2A	3641	1/1	0.72	0.53	57,57,57,57	0
55	MG	2A	3819	1/1	0.73	0.80	55,55,55,55	0
55	MG	2A	3542	1/1	0.73	0.27	66,66,66,66	0
55	MG	2a	1655	1/1	0.73	0.36	62,62,62,62	0
55	MG	1A	3320	1/1	0.73	0.13	44,44,44,44	0
55	MG	2B	3010	1/1	0.73	0.19	70,70,70,70	0
55	MG	2A	3744	1/1	0.73	0.17	58,58,58,58	0
55	MG	1a	1653	1/1	0.73	0.36	43,43,43,43	0
55	MG	2A	3690	1/1	0.73	0.24	43,43,43,43	0
55	MG	1A	3081	1/1	0.73	0.70	41,41,41,41	0
55	MG	2A	3599	1/1	0.73	0.40	52,52,52,52	0
55	MG	2A	3944	1/1	0.73	0.58	57,57,57,57	0
55	MG	2A	3726	1/1	0.73	0.37	73,73,73,73	0
55	MG	2a	1635	1/1	0.73	0.41	63,63,63,63	0
55	MG	2A	3586	1/1	0.74	0.26	35,35,35,35	0
55	MG	2A	3259	1/1	0.74	0.15	82,82,82,82	0
55	MG	1a	1626	1/1	0.74	0.30	47,47,47,47	0
55	MG	1a	1669	1/1	0.74	0.42	61,61,61,61	0
55	MG	1A	3602	1/1	0.74	0.54	46,46,46,46	0
55	MG	2a	1668	1/1	0.74	1.39	60,60,60,60	0
55	MG	2A	3931	1/1	0.74	0.98	63,63,63,63	0
55	MG	2A	3025	1/1	0.74	1.08	42,42,42,42	0
55	MG	1Q	203	1/1	0.74	0.40	40,40,40,40	0
55	MG	1A	3493	1/1	0.74	0.48	44,44,44,44	0
55	MG	2A	3199	1/1	0.74	0.74	32,32,32,32	0
55	MG	1A	3589	1/1	0.74	0.16	72,72,72,72	0
55	MG	2a	1650	1/1	0.74	0.20	51,51,51,51	0
55	MG	1A	3718	1/1	0.75	0.34	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3626	1/1	0.75	0.37	64,64,64,64	0
55	MG	1A	3780	1/1	0.75	0.41	39,39,39,39	0
55	MG	1a	1837	1/1	0.75	0.24	93,93,93,93	0
55	MG	1A	3699	1/1	0.75	0.33	47,47,47,47	0
55	MG	1d	303	1/1	0.75	0.42	59,59,59,59	0
55	MG	2A	3152	1/1	0.75	0.58	36,36,36,36	0
55	MG	2A	3828	1/1	0.75	0.20	88,88,88,88	0
55	MG	2d	504	1/1	0.75	0.44	66,66,66,66	0
55	MG	1A	3946	1/1	0.75	0.48	40,40,40,40	0
55	MG	2A	3595	1/1	0.75	0.28	79,79,79,79	0
55	MG	1A	3032	1/1	0.75	0.77	30,30,30,30	0
55	MG	2S	201	1/1	0.75	0.27	46,46,46,46	0
55	MG	1A	3219	1/1	0.76	0.30	30,30,30,30	0
55	MG	1A	3621	1/1	0.76	0.35	58,58,58,58	0
55	MG	1a	1643	1/1	0.76	0.28	61,61,61,61	0
55	MG	2A	3008	1/1	0.76	0.29	40,40,40,40	0
55	MG	2a	1827	1/1	0.76	0.56	77,77,77,77	0
55	MG	29	104	1/1	0.76	0.99	75,75,75,75	0
55	MG	1A	3638	1/1	0.76	0.43	49,49,49,49	0
55	MG	2a	1832	1/1	0.76	0.39	83,83,83,83	0
55	MG	2A	3033	1/1	0.76	0.40	44,44,44,44	0
55	MG	2a	1617	1/1	0.76	0.94	83,83,83,83	0
55	MG	1B	227	1/1	0.76	0.38	29,29,29,29	0
55	MG	2a	1719	1/1	0.76	0.14	76,76,76,76	0
55	MG	1A	3122	1/1	0.76	0.53	39,39,39,39	0
55	MG	1A	3274	1/1	0.76	0.37	79,79,79,79	0
55	MG	2A	3250	1/1	0.76	0.72	54,54,54,54	0
55	MG	2A	3098	1/1	0.76	0.65	50,50,50,50	0
55	MG	23	102	1/1	0.77	1.09	59,59,59,59	0
55	MG	29	101	1/1	0.77	0.41	46,46,46,46	0
55	MG	2B	3011	1/1	0.77	0.22	89,89,89,89	0
55	MG	2A	3031	1/1	0.77	0.37	45,45,45,45	0
55	MG	2B	3015	1/1	0.77	0.22	62,62,62,62	0
55	MG	2A	3907	1/1	0.77	0.67	56,56,56,56	0
55	MG	2A	3596	1/1	0.77	0.11	68,68,68,68	0
55	MG	1A	3550	1/1	0.77	0.31	36,36,36,36	0
55	MG	2A	3751	1/1	0.77	0.60	77,77,77,77	0
55	MG	2a	1640	1/1	0.77	0.77	60,60,60,60	0
55	MG	1F	304	1/1	0.77	0.18	31,31,31,31	0
55	MG	2A	3515	1/1	0.77	0.35	68,68,68,68	0
55	MG	1A	3074	1/1	0.77	0.64	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1A	3046	1/1	0.77	0.38	40,40,40,40	0
55	MG	1a	1602	1/1	0.77	0.08	78,78,78,78	0
55	MG	2G	3002	1/1	0.77	0.09	71,71,71,71	0
55	MG	2A	3961	1/1	0.77	0.39	52,52,52,52	0
55	MG	1A	3783	1/1	0.77	0.39	67,67,67,67	0
55	MG	2A	3022	1/1	0.77	0.42	49,49,49,49	0
55	MG	2t	201	1/1	0.77	0.21	75,75,75,75	0
55	MG	2A	3850	1/1	0.77	0.13	81,81,81,81	0
55	MG	1a	1832	1/1	0.77	0.10	104,104,104,104	0
55	MG	1A	3040	1/1	0.78	0.44	39,39,39,39	0
55	MG	2A	3710	1/1	0.78	0.19	40,40,40,40	0
55	MG	2A	3230	1/1	0.78	0.59	49,49,49,49	0
55	MG	1A	3481	1/1	0.78	0.20	56,56,56,56	0
55	MG	1A	3846	1/1	0.78	0.19	29,29,29,29	0
55	MG	2a	1755	1/1	0.78	0.26	99,99,99,99	0
55	MG	1a	1668	1/1	0.78	0.33	60,60,60,60	0
55	MG	2A	3594	1/1	0.78	0.73	43,43,43,43	0
55	MG	1A	3119	1/1	0.78	0.28	35,35,35,35	0
55	MG	2a	1639	1/1	0.78	0.58	63,63,63,63	0
55	MG	2A	3929	1/1	0.78	0.75	58,58,58,58	0
55	MG	2A	3178	1/1	0.78	0.34	37,37,37,37	0
55	MG	2a	1646	1/1	0.78	0.09	76,76,76,76	0
55	MG	2A	3378	1/1	0.78	0.16	72,72,72,72	0
55	MG	2A	3941	1/1	0.78	0.59	104,104,104,104	0
55	MG	2A	3413	1/1	0.78	0.49	36,36,36,36	0
55	MG	1A	3918	1/1	0.78	0.30	35,35,35,35	0
55	MG	2A	3795	1/1	0.78	0.83	42,42,42,42	0
55	MG	2A	3969	1/1	0.78	1.10	53,53,53,53	0
55	MG	2B	3005	1/1	0.78	0.37	74,74,74,74	0
55	MG	1A	3729	1/1	0.78	0.18	95,95,95,95	0
55	MG	1a	1806	1/1	0.78	0.40	74,74,74,74	0
55	MG	2A	3532	1/1	0.78	0.14	56,56,56,56	0
55	MG	2a	1684	1/1	0.79	0.34	53,53,53,53	0
55	MG	1A	3914	1/1	0.79	0.20	40,40,40,40	0
55	MG	2A	3650	1/1	0.79	0.45	71,71,71,71	0
55	MG	2a	1736	1/1	0.79	0.31	46,46,46,46	0
55	MG	2A	3487	1/1	0.79	0.33	52,52,52,52	0
55	MG	1A	3562	1/1	0.79	0.41	63,63,63,63	0
55	MG	1i	3001	1/1	0.79	0.26	74,74,74,74	0
55	MG	1A	3584	1/1	0.79	0.83	32,32,32,32	0
55	MG	2A	3232	1/1	0.79	0.44	44,44,44,44	0
55	MG	2a	1631	1/1	0.79	1.53	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1a	1779	1/1	0.79	0.15	81,81,81,81	0
55	MG	2A	3567	1/1	0.79	0.35	53,53,53,53	0
55	MG	2A	3930	1/1	0.79	0.26	61,61,61,61	0
55	MG	2A	3123	1/1	0.79	0.30	49,49,49,49	0
55	MG	1A	3812	1/1	0.79	0.24	96,96,96,96	0
55	MG	2A	3262	1/1	0.79	0.39	51,51,51,51	0
55	MG	2F	310	1/1	0.79	0.44	40,40,40,40	0
55	MG	1A	3173	1/1	0.79	0.45	49,49,49,49	0
55	MG	1a	1750	1/1	0.79	0.25	68,68,68,68	0
55	MG	1A	3184	1/1	0.79	0.57	33,33,33,33	0
55	MG	2A	3394	1/1	0.79	0.13	72,72,72,72	0
55	MG	2B	3003	1/1	0.79	0.17	67,67,67,67	0
55	MG	2A	3404	1/1	0.79	0.46	78,78,78,78	0
55	MG	1a	1640	1/1	0.79	0.61	58,58,58,58	0
55	MG	2A	3417	1/1	0.79	0.19	46,46,46,46	0
55	MG	2A	3628	1/1	0.80	0.39	79,79,79,79	0
55	MG	1l	3001	1/1	0.80	0.13	59,59,59,59	0
55	MG	1A	3660	1/1	0.80	0.45	55,55,55,55	0
55	MG	2D	316	1/1	0.80	0.74	58,58,58,58	0
55	MG	2A	3177	1/1	0.80	0.40	42,42,42,42	0
55	MG	2a	1676	1/1	0.80	0.26	102,102,102,102	0
55	MG	17	101	1/1	0.80	0.77	34,34,34,34	0
55	MG	2A	3452	1/1	0.80	0.15	82,82,82,82	0
55	MG	1a	1778	1/1	0.80	0.18	92,92,92,92	0
55	MG	2A	3508	1/1	0.80	0.40	59,59,59,59	0
55	MG	2A	3938	1/1	0.80	0.28	46,46,46,46	0
55	MG	19	101	1/1	0.80	0.35	24,24,24,24	0
55	MG	1a	1647	1/1	0.80	0.11	65,65,65,65	0
55	MG	1a	1807	1/1	0.80	0.11	98,98,98,98	0
55	MG	1a	1810	1/1	0.80	0.18	81,81,81,81	0
55	MG	1A	3264	1/1	0.80	0.35	58,58,58,58	0
55	MG	2A	3068	1/1	0.80	0.90	39,39,39,39	0
55	MG	1a	1740	1/1	0.80	0.26	81,81,81,81	0
55	MG	1a	1748	1/1	0.80	0.13	86,86,86,86	0
55	MG	2A	3782	1/1	0.80	0.47	58,58,58,58	0
55	MG	1A	3138	1/1	0.80	0.10	52,52,52,52	0
55	MG	2a	1625	1/1	0.80	0.36	59,59,59,59	0
55	MG	1B	211	1/1	0.80	0.42	58,58,58,58	0
55	MG	2A	3302	1/1	0.80	0.22	51,51,51,51	0
55	MG	1a	1628	1/1	0.80	0.20	38,38,38,38	0
55	MG	2A	3347	1/1	0.80	0.15	44,44,44,44	0
55	MG	2A	3615	1/1	0.80	0.20	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	2A	3868	1/1	0.80	0.38	106,106,106,106	0
55	MG	2A	3874	1/1	0.80	0.39	67,67,67,67	0
55	MG	2A	3130	1/1	0.80	0.21	41,41,41,41	0
55	MG	2t	202	1/1	0.80	0.38	72,72,72,72	0
55	MG	1a	1632	1/1	0.80	1.21	57,57,57,57	0
55	MG	2A	3891	1/1	0.80	0.14	72,72,72,72	0
55	MG	2A	3040	1/1	0.81	0.42	51,51,51,51	0
55	MG	1a	1608	1/1	0.81	0.40	74,74,74,74	0
55	MG	1A	3411	1/1	0.81	0.19	51,51,51,51	0
55	MG	1A	3269	1/1	0.81	0.48	49,49,49,49	0
55	MG	1a	1756	1/1	0.81	0.23	75,75,75,75	0
55	MG	2a	1658	1/1	0.81	0.21	83,83,83,83	0
55	MG	2a	1660	1/1	0.81	0.48	42,42,42,42	0
55	MG	2a	1661	1/1	0.81	0.35	60,60,60,60	0
55	MG	1A	3224	1/1	0.81	0.41	32,32,32,32	0
55	MG	1a	1838	1/1	0.81	0.49	27,27,27,27	0
55	MG	2A	3857	1/1	0.81	0.68	47,47,47,47	0
55	MG	1a	1841	1/1	0.81	0.25	52,52,52,52	0
55	MG	2A	3619	1/1	0.81	0.31	74,74,74,74	0
55	MG	2A	3884	1/1	0.81	0.08	65,65,65,65	0
55	MG	1a	1845	1/1	0.81	0.99	107,107,107,107	0
55	MG	1A	3297	1/1	0.81	0.64	34,34,34,34	0
55	MG	2E	305	1/1	0.81	0.29	53,53,53,53	0
55	MG	2a	1686	1/1	0.81	0.10	78,78,78,78	0
55	MG	2A	3146	1/1	0.81	0.32	68,68,68,68	0
55	MG	2a	1721	1/1	0.81	0.43	84,84,84,84	0
55	MG	1a	1765	1/1	0.81	0.35	81,81,81,81	0
55	MG	1A	3494	1/1	0.81	0.13	28,28,28,28	0
55	MG	1A	3231	1/1	0.81	0.39	40,40,40,40	0
55	MG	2A	3679	1/1	0.81	0.23	60,60,60,60	0
55	MG	2a	1751	1/1	0.81	0.20	93,93,93,93	0
55	MG	2A	3689	1/1	0.81	0.20	37,37,37,37	0
55	MG	20	101	1/1	0.81	0.54	48,48,48,48	0
55	MG	2a	1764	1/1	0.81	0.30	67,67,67,67	0
55	MG	1A	3623	1/1	0.81	0.15	59,59,59,59	0
55	MG	2A	3473	1/1	0.81	0.19	66,66,66,66	0
55	MG	20	105	1/1	0.81	0.99	62,62,62,62	0
55	MG	2a	1809	1/1	0.81	0.15	68,68,68,68	0
55	MG	2A	3006	1/1	0.81	0.40	42,42,42,42	0
55	MG	2A	3502	1/1	0.81	0.09	69,69,69,69	0
55	MG	2A	3007	1/1	0.81	0.28	59,59,59,59	0
55	MG	2A	3511	1/1	0.81	0.30	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1A	3325	1/1	0.81	0.28	29,29,29,29	0
55	MG	2A	3742	1/1	0.81	0.19	52,52,52,52	0
55	MG	1a	1789	1/1	0.81	0.15	117,117,117,117	0
55	MG	1a	1791	1/1	0.81	0.36	64,64,64,64	0
55	MG	1a	1704	1/1	0.81	0.25	67,67,67,67	0
55	MG	2a	1627	1/1	0.81	0.27	25,25,25,25	0
55	MG	1B	204	1/1	0.81	0.14	63,63,63,63	0
55	MG	2o	101	1/1	0.81	0.29	66,66,66,66	0
55	MG	2A	3765	1/1	0.81	0.32	67,67,67,67	0
55	MG	2a	1636	1/1	0.81	1.08	63,63,63,63	0
55	MG	2A	3779	1/1	0.81	0.15	60,60,60,60	0
55	MG	2A	3235	1/1	0.81	0.28	63,63,63,63	0
55	MG	1a	1788	1/1	0.82	0.06	70,70,70,70	0
55	MG	1A	3265	1/1	0.82	0.51	43,43,43,43	0
55	MG	2A	3350	1/1	0.82	0.13	40,40,40,40	0
55	MG	2A	3605	1/1	0.82	0.17	55,55,55,55	0
55	MG	2A	3845	1/1	0.82	0.92	42,42,42,42	0
55	MG	2A	3608	1/1	0.82	0.30	48,48,48,48	0
55	MG	2a	1670	1/1	0.82	0.22	56,56,56,56	0
55	MG	2A	3004	1/1	0.82	0.27	54,54,54,54	0
55	MG	2A	3618	1/1	0.82	0.16	83,83,83,83	0
55	MG	1a	1744	1/1	0.82	0.55	64,64,64,64	0
55	MG	2a	1677	1/1	0.82	0.20	68,68,68,68	0
55	MG	1B	215	1/1	0.82	0.45	50,50,50,50	0
55	MG	1A	3762	1/1	0.82	0.23	50,50,50,50	0
55	MG	1a	1809	1/1	0.82	0.11	85,85,85,85	0
55	MG	2a	1697	1/1	0.82	0.13	66,66,66,66	0
55	MG	2a	1702	1/1	0.82	0.22	52,52,52,52	0
55	MG	2A	3640	1/1	0.82	0.11	72,72,72,72	0
55	MG	1a	1751	1/1	0.82	0.18	98,98,98,98	0
55	MG	2A	3421	1/1	0.82	0.09	54,54,54,54	0
55	MG	1A	3778	1/1	0.82	0.51	46,46,46,46	0
55	MG	2A	3916	1/1	0.82	1.27	48,48,48,48	0
55	MG	2A	3667	1/1	0.82	0.22	89,89,89,89	0
55	MG	2A	3677	1/1	0.82	0.35	48,48,48,48	0
55	MG	2A	3459	1/1	0.82	0.09	53,53,53,53	0
55	MG	1a	1754	1/1	0.82	0.19	66,66,66,66	0
55	MG	2A	3038	1/1	0.82	0.39	46,46,46,46	0
55	MG	2a	1605	1/1	0.82	0.30	82,82,82,82	0
55	MG	2a	1607	1/1	0.82	0.23	49,49,49,49	0
55	MG	2A	3495	1/1	0.82	0.09	42,42,42,42	0
55	MG	2a	1806	1/1	0.82	0.23	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	1833	1/1	0.82	0.21	98,98,98,98	0
55	MG	1D	311	1/1	0.82	0.16	43,43,43,43	0
55	MG	2A	3233	1/1	0.82	0.28	56,56,56,56	0
55	MG	2A	3513	1/1	0.82	0.30	66,66,66,66	0
55	MG	1A	3174	1/1	0.82	0.15	40,40,40,40	0
55	MG	2A	3245	1/1	0.82	0.38	54,54,54,54	0
55	MG	2A	3971	1/1	0.82	0.31	73,73,73,73	0
55	MG	2A	3524	1/1	0.82	0.52	74,74,74,74	0
55	MG	1A	3940	1/1	0.82	0.64	51,51,51,51	0
55	MG	1a	1641	1/1	0.82	0.40	37,37,37,37	0
55	MG	2A	3754	1/1	0.82	0.37	39,39,39,39	0
55	MG	1a	1679	1/1	0.82	0.19	46,46,46,46	0
55	MG	1A	3239	1/1	0.82	0.21	46,46,46,46	0
55	MG	1A	3786	1/1	0.82	0.08	65,65,65,65	0
55	MG	2A	3299	1/1	0.82	0.27	44,44,44,44	0
55	MG	1A	3724	1/1	0.82	0.77	47,47,47,47	0
55	MG	2A	3311	1/1	0.82	0.11	66,66,66,66	0
55	MG	1d	304	1/1	0.83	0.26	68,68,68,68	0
55	MG	2A	3492	1/1	0.83	1.07	41,41,41,41	0
55	MG	2A	3734	1/1	0.83	0.20	81,81,81,81	0
55	MG	1B	208	1/1	0.83	0.14	41,41,41,41	0
55	MG	2A	3179	1/1	0.83	0.59	39,39,39,39	0
55	MG	2a	1722	1/1	0.83	0.20	52,52,52,52	0
55	MG	2a	1621	1/1	0.83	0.24	82,82,82,82	0
55	MG	2B	3018	1/1	0.83	0.13	70,70,70,70	0
55	MG	1a	1681	1/1	0.83	0.40	59,59,59,59	0
55	MG	1A	3372	1/1	0.83	0.19	68,68,68,68	0
55	MG	1A	3878	1/1	0.83	0.42	49,49,49,49	0
55	MG	1A	3744	1/1	0.83	0.19	29,29,29,29	0
55	MG	2A	3226	1/1	0.83	0.42	41,41,41,41	0
55	MG	1a	1615	1/1	0.83	0.18	72,72,72,72	0
55	MG	1A	3271	1/1	0.83	0.91	29,29,29,29	0
55	MG	2A	3009	1/1	0.83	0.32	31,31,31,31	0
55	MG	2a	1784	1/1	0.83	0.12	125,125,125,125	0
55	MG	2A	3557	1/1	0.83	0.28	77,77,77,77	0
55	MG	2A	3783	1/1	0.83	0.35	42,42,42,42	0
55	MG	2A	3658	1/1	0.83	0.45	45,45,45,45	0
55	MG	1A	3313	1/1	0.83	0.31	41,41,41,41	0
55	MG	2N	202	1/1	0.83	0.43	64,64,64,64	0
55	MG	2P	202	1/1	0.83	0.24	84,84,84,84	0
55	MG	2A	3950	1/1	0.83	0.19	55,55,55,55	0
55	MG	2W	3003	1/1	0.83	0.46	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2X	101	1/1	0.83	0.79	64,64,64,64	0
55	MG	1A	3080	1/1	0.83	0.43	22,22,22,22	0
55	MG	2a	1842	1/1	0.83	0.52	71,71,71,71	0
55	MG	1A	3290	1/1	0.83	0.27	21,21,21,21	0
55	MG	2a	1669	1/1	0.83	0.17	56,56,56,56	0
55	MG	2A	3434	1/1	0.83	0.13	39,39,39,39	0
55	MG	2h	3002	1/1	0.83	0.59	73,73,73,73	0
55	MG	2A	3439	1/1	0.83	0.10	50,50,50,50	0
55	MG	2A	3155	1/1	0.83	0.34	45,45,45,45	0
55	MG	2A	3701	1/1	0.83	0.49	60,60,60,60	0
55	MG	1A	3574	1/1	0.83	0.21	49,49,49,49	0
55	MG	1A	3645	1/1	0.83	0.47	45,45,45,45	0
55	MG	2A	3721	1/1	0.83	0.32	47,47,47,47	0
55	MG	2A	3159	1/1	0.84	0.31	45,45,45,45	0
55	MG	2a	1664	1/1	0.84	0.71	80,80,80,80	0
55	MG	1a	1635	1/1	0.84	0.20	46,46,46,46	0
55	MG	2A	3169	1/1	0.84	0.58	54,54,54,54	0
55	MG	2A	3380	1/1	0.84	0.06	35,35,35,35	0
55	MG	2D	312	1/1	0.84	0.30	48,48,48,48	0
55	MG	2A	3174	1/1	0.84	0.41	36,36,36,36	0
55	MG	1A	3199	1/1	0.84	0.24	44,44,44,44	0
55	MG	1A	3603	1/1	0.84	0.13	48,48,48,48	0
55	MG	1A	3152	1/1	0.84	0.22	37,37,37,37	0
55	MG	2E	306	1/1	0.84	0.16	35,35,35,35	0
55	MG	2A	3027	1/1	0.84	0.13	42,42,42,42	0
55	MG	2A	3624	1/1	0.84	0.75	56,56,56,56	0
55	MG	1A	3455	1/1	0.84	0.20	89,89,89,89	0
55	MG	2A	3872	1/1	0.84	0.20	71,71,71,71	0
55	MG	1A	3899	1/1	0.84	0.17	68,68,68,68	0
55	MG	2A	3881	1/1	0.84	0.48	49,49,49,49	0
55	MG	2A	3630	1/1	0.84	0.13	73,73,73,73	0
55	MG	2A	3631	1/1	0.84	0.11	75,75,75,75	0
55	MG	1F	308	1/1	0.84	0.61	39,39,39,39	0
55	MG	1A	3723	1/1	0.84	0.33	63,63,63,63	0
55	MG	2A	3206	1/1	0.84	0.25	54,54,54,54	0
55	MG	2A	3461	1/1	0.84	0.23	88,88,88,88	0
55	MG	2A	3655	1/1	0.84	0.54	53,53,53,53	0
55	MG	2a	1752	1/1	0.84	0.14	77,77,77,77	0
55	MG	2A	3207	1/1	0.84	0.66	58,58,58,58	0
55	MG	1U	201	1/1	0.84	0.29	26,26,26,26	0
55	MG	2A	3490	1/1	0.84	0.20	68,68,68,68	0
55	MG	2A	3049	1/1	0.84	0.48	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3680	1/1	0.84	0.16	53,53,53,53	0
55	MG	1A	3009	1/1	0.84	0.31	19,19,19,19	0
55	MG	1A	3916	1/1	0.84	0.07	116,116,116,116	0
55	MG	1A	3033	1/1	0.84	0.20	49,49,49,49	0
55	MG	1A	3646	1/1	0.84	0.32	38,38,38,38	0
55	MG	2A	3708	1/1	0.84	0.14	63,63,63,63	0
55	MG	2A	3248	1/1	0.84	0.28	44,44,44,44	0
55	MG	2A	3106	1/1	0.84	0.34	43,43,43,43	0
55	MG	1A	3649	1/1	0.84	0.23	40,40,40,40	0
55	MG	1A	3133	1/1	0.84	0.55	47,47,47,47	0
55	MG	1B	203	1/1	0.84	0.23	46,46,46,46	0
55	MG	2A	3271	1/1	0.84	0.23	34,34,34,34	0
55	MG	2A	3553	1/1	0.84	0.11	51,51,51,51	0
55	MG	2A	3556	1/1	0.84	0.28	65,65,65,65	0
55	MG	1A	3654	1/1	0.84	0.22	35,35,35,35	0
55	MG	2A	3142	1/1	0.84	0.14	78,78,78,78	0
55	MG	2h	3001	1/1	0.84	0.34	43,43,43,43	0
55	MG	1A	3782	1/1	0.84	0.35	60,60,60,60	0
55	MG	2A	3568	1/1	0.84	0.70	53,53,53,53	0
55	MG	1a	1799	1/1	0.84	0.06	73,73,73,73	0
55	MG	1A	3096	1/1	0.84	0.26	48,48,48,48	0
55	MG	2A	3776	1/1	0.84	1.21	69,69,69,69	0
55	MG	2A	3332	1/1	0.84	0.13	61,61,61,61	0
55	MG	2A	3335	1/1	0.84	0.13	77,77,77,77	0
55	MG	1a	1758	1/1	0.85	0.16	99,99,99,99	0
55	MG	2A	3555	1/1	0.85	0.28	54,54,54,54	0
55	MG	2a	1620	1/1	0.85	0.29	58,58,58,58	0
55	MG	1A	3722	1/1	0.85	0.20	49,49,49,49	0
55	MG	2a	1735	1/1	0.85	0.16	87,87,87,87	0
55	MG	2A	3200	1/1	0.85	0.51	41,41,41,41	0
55	MG	2A	3456	1/1	0.85	0.14	62,62,62,62	0
55	MG	2A	3029	1/1	0.85	0.24	39,39,39,39	0
55	MG	2a	1749	1/1	0.85	0.23	75,75,75,75	0
55	MG	2A	3648	1/1	0.85	0.12	49,49,49,49	0
55	MG	1A	3161	1/1	0.85	0.66	26,26,26,26	0
55	MG	1A	3673	1/1	0.85	0.86	40,40,40,40	0
55	MG	2A	3330	1/1	0.85	0.10	78,78,78,78	0
55	MG	2A	3777	1/1	0.85	0.48	63,63,63,63	0
55	MG	2a	1767	1/1	0.85	0.35	74,74,74,74	0
55	MG	1a	1741	1/1	0.85	0.38	42,42,42,42	0
55	MG	2A	3673	1/1	0.85	0.19	58,58,58,58	0
55	MG	2A	3675	1/1	0.85	0.49	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3676	1/1	0.85	0.22	62,62,62,62	0
55	MG	1A	3466	1/1	0.85	0.24	36,36,36,36	0
55	MG	2A	3231	1/1	0.85	0.13	59,59,59,59	0
55	MG	2A	3001	1/1	0.85	0.13	47,47,47,47	0
55	MG	2A	3951	1/1	0.85	0.71	38,38,38,38	0
55	MG	1A	3809	1/1	0.85	0.11	63,63,63,63	0
55	MG	2A	3603	1/1	0.85	0.23	59,59,59,59	0
55	MG	2A	3833	1/1	0.85	0.20	44,44,44,44	0
55	MG	2A	3842	1/1	0.85	0.23	65,65,65,65	0
55	MG	1A	3518	1/1	0.85	0.12	50,50,50,50	0
55	MG	1A	3127	1/1	0.85	0.18	34,34,34,34	0
55	MG	2B	3007	1/1	0.85	0.12	52,52,52,52	0
55	MG	1a	1609	1/1	0.85	0.27	80,80,80,80	0
55	MG	2e	201	1/1	0.85	0.21	57,57,57,57	0
55	MG	1A	3873	1/1	0.85	0.34	20,20,20,20	0
55	MG	2A	3100	1/1	0.85	0.24	56,56,56,56	0
55	MG	2A	3010	1/1	0.85	0.56	49,49,49,49	0
55	MG	2A	3875	1/1	0.85	0.66	102,102,102,102	0
55	MG	2a	1612	1/1	0.85	0.27	42,42,42,42	0
55	MG	1A	3175	1/1	0.85	0.15	50,50,50,50	0
55	MG	2A	3543	1/1	0.85	0.28	57,57,57,57	0
55	MG	2a	1616	1/1	0.85	0.20	69,69,69,69	0
55	MG	2a	1717	1/1	0.85	0.29	90,90,90,90	0
55	MG	1A	3789	1/1	0.86	0.09	42,42,42,42	0
55	MG	1A	3804	1/1	0.86	0.48	26,26,26,26	0
55	MG	2A	3620	1/1	0.86	0.98	65,65,65,65	0
55	MG	1A	3691	1/1	0.86	0.12	39,39,39,39	0
55	MG	1A	3613	1/1	0.86	0.11	53,53,53,53	0
55	MG	1D	315	1/1	0.86	0.18	68,68,68,68	0
55	MG	1A	3616	1/1	0.86	0.11	38,38,38,38	0
55	MG	2a	1673	1/1	0.86	0.20	61,61,61,61	0
55	MG	2A	3849	1/1	0.86	0.27	64,64,64,64	0
55	MG	1a	1772	1/1	0.86	0.20	71,71,71,71	0
55	MG	1a	1775	1/1	0.86	0.21	68,68,68,68	0
55	MG	2A	3861	1/1	0.86	0.16	50,50,50,50	0
55	MG	1a	1777	1/1	0.86	0.08	72,72,72,72	0
55	MG	2a	1694	1/1	0.86	0.20	53,53,53,53	0
55	MG	1A	3864	1/1	0.86	0.56	51,51,51,51	0
55	MG	2A	3469	1/1	0.86	0.32	58,58,58,58	0
55	MG	1A	3532	1/1	0.86	0.24	68,68,68,68	0
55	MG	1a	1785	1/1	0.86	0.17	96,96,96,96	0
55	MG	2V	204	1/1	0.86	0.54	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3030	1/1	0.86	0.37	23,23,23,23	0
55	MG	2A	3218	1/1	0.86	0.53	45,45,45,45	0
55	MG	1A	3198	1/1	0.86	0.14	67,67,67,67	0
55	MG	2A	3670	1/1	0.86	0.26	57,57,57,57	0
55	MG	2A	3672	1/1	0.86	0.19	65,65,65,65	0
55	MG	1a	1670	1/1	0.86	0.19	55,55,55,55	0
55	MG	2A	3504	1/1	0.86	0.73	71,71,71,71	0
55	MG	1A	3879	1/1	0.86	0.44	33,33,33,33	0
55	MG	25	103	1/1	0.86	0.71	49,49,49,49	0
55	MG	2A	3510	1/1	0.86	0.12	43,43,43,43	0
55	MG	2A	3919	1/1	0.86	0.21	122,122,122,122	0
55	MG	2a	1759	1/1	0.86	0.25	84,84,84,84	0
55	MG	1a	1673	1/1	0.86	0.27	35,35,35,35	0
55	MG	1a	1674	1/1	0.86	0.26	68,68,68,68	0
55	MG	1A	3882	1/1	0.86	0.11	56,56,56,56	0
55	MG	2A	3519	1/1	0.86	0.15	51,51,51,51	0
55	MG	1a	1677	1/1	0.86	0.36	102,102,102,102	0
55	MG	2A	3061	1/1	0.86	0.19	39,39,39,39	0
55	MG	18	3301	1/1	0.86	0.54	45,45,45,45	0
55	MG	2a	1808	1/1	0.86	0.29	76,76,76,76	0
55	MG	2A	3251	1/1	0.86	0.28	60,60,60,60	0
55	MG	1A	3634	1/1	0.86	0.14	34,34,34,34	0
55	MG	2A	3083	1/1	0.86	1.06	35,35,35,35	0
55	MG	2A	3554	1/1	0.86	0.17	67,67,67,67	0
55	MG	1A	3172	1/1	0.86	0.32	52,52,52,52	0
55	MG	1A	3073	1/1	0.86	0.22	36,36,36,36	0
55	MG	1A	3733	1/1	0.86	0.11	37,37,37,37	0
55	MG	1A	3566	1/1	0.86	0.11	52,52,52,52	0
55	MG	2A	3112	1/1	0.86	1.11	32,32,32,32	0
55	MG	1A	3258	1/1	0.86	0.21	38,38,38,38	0
55	MG	2A	3320	1/1	0.86	0.10	72,72,72,72	0
55	MG	1A	3763	1/1	0.86	0.13	40,40,40,40	0
55	MG	1A	3580	1/1	0.86	0.32	26,26,26,26	0
55	MG	2A	3132	1/1	0.86	0.24	36,36,36,36	0
55	MG	1a	1629	1/1	0.86	0.58	51,51,51,51	0
55	MG	1A	3146	1/1	0.86	0.45	22,22,22,22	0
55	MG	2l	3002	1/1	0.86	0.19	70,70,70,70	0
55	MG	2A	3151	1/1	0.86	0.36	37,37,37,37	0
55	MG	1A	3163	1/1	0.86	0.67	32,32,32,32	0
55	MG	1f	8001	1/1	0.86	0.36	68,68,68,68	0
55	MG	1A	3233	1/1	0.86	0.40	33,33,33,33	0
55	MG	1A	3148	1/1	0.86	0.38	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3257	1/1	0.87	0.20	47,47,47,47	0
55	MG	1A	3182	1/1	0.87	0.28	24,24,24,24	0
55	MG	1a	1601	1/1	0.87	0.16	45,45,45,45	0
55	MG	2A	3763	1/1	0.87	0.44	61,61,61,61	0
55	MG	2A	3261	1/1	0.87	0.19	39,39,39,39	0
55	MG	2A	3097	1/1	0.87	0.68	69,69,69,69	0
55	MG	1A	3900	1/1	0.87	0.15	32,32,32,32	0
55	MG	1A	3636	1/1	0.87	0.54	40,40,40,40	0
55	MG	1a	1715	1/1	0.87	0.14	58,58,58,58	0
55	MG	2A	3585	1/1	0.87	0.26	65,65,65,65	0
55	MG	2D	303	1/1	0.87	0.27	41,41,41,41	0
55	MG	1A	3538	1/1	0.87	0.22	48,48,48,48	0
55	MG	2A	3110	1/1	0.87	0.71	58,58,58,58	0
55	MG	1A	3151	1/1	0.87	0.16	20,20,20,20	0
55	MG	2a	1681	1/1	0.87	0.18	54,54,54,54	0
55	MG	1A	3041	1/1	0.87	0.14	26,26,26,26	0
55	MG	2A	3120	1/1	0.87	0.07	54,54,54,54	0
55	MG	2A	3811	1/1	0.87	0.20	65,65,65,65	0
55	MG	1a	1746	1/1	0.87	0.12	55,55,55,55	0
55	MG	1A	3938	1/1	0.87	0.89	21,21,21,21	0
55	MG	2a	1709	1/1	0.87	0.29	102,102,102,102	0
55	MG	1A	3027	1/1	0.87	0.23	46,46,46,46	0
55	MG	2A	3137	1/1	0.87	0.29	36,36,36,36	0
55	MG	2A	3359	1/1	0.87	0.10	34,34,34,34	0
55	MG	2A	3370	1/1	0.87	0.24	76,76,76,76	0
55	MG	1d	306	1/1	0.87	0.06	98,98,98,98	0
55	MG	1A	3132	1/1	0.87	0.24	22,22,22,22	0
55	MG	1a	1630	1/1	0.87	0.30	42,42,42,42	0
55	MG	2A	3867	1/1	0.87	0.15	58,58,58,58	0
55	MG	1k	3001	1/1	0.87	0.13	53,53,53,53	0
55	MG	1A	3651	1/1	0.87	0.10	37,37,37,37	0
55	MG	1A	3781	1/1	0.87	0.27	28,28,28,28	0
55	MG	1o	102	1/1	0.87	0.26	29,29,29,29	0
55	MG	1A	3467	1/1	0.87	0.11	23,23,23,23	0
55	MG	1A	3166	1/1	0.87	0.22	33,33,33,33	0
55	MG	1A	3669	1/1	0.87	0.12	47,47,47,47	0
55	MG	2A	3441	1/1	0.87	0.10	87,87,87,87	0
55	MG	1A	3672	1/1	0.87	0.11	44,44,44,44	0
55	MG	1A	3002	1/1	0.87	0.44	49,49,49,49	0
55	MG	1A	3486	1/1	0.87	0.12	35,35,35,35	0
55	MG	2a	1606	1/1	0.87	0.11	53,53,53,53	0
55	MG	2A	3182	1/1	0.87	0.47	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3462	1/1	0.87	0.56	59,59,59,59	0
55	MG	1A	3054	1/1	0.87	0.23	34,34,34,34	0
55	MG	2A	3011	1/1	0.87	0.28	54,54,54,54	0
55	MG	2a	1810	1/1	0.87	0.10	105,105,105,105	0
55	MG	1A	3144	1/1	0.87	0.31	29,29,29,29	0
55	MG	1A	3855	1/1	0.87	0.29	37,37,37,37	0
55	MG	2A	3201	1/1	0.87	0.20	71,71,71,71	0
55	MG	1A	3715	1/1	0.87	0.17	16,16,16,16	0
55	MG	1P	204	1/1	0.87	0.16	68,68,68,68	0
55	MG	1A	3866	1/1	0.87	0.09	79,79,79,79	0
55	MG	2A	3212	1/1	0.87	0.51	51,51,51,51	0
55	MG	1a	1671	1/1	0.87	0.21	49,49,49,49	0
55	MG	2A	3032	1/1	0.87	1.01	51,51,51,51	0
55	MG	2a	1634	1/1	0.87	0.30	59,59,59,59	0
55	MG	1A	3501	1/1	0.87	0.26	31,31,31,31	0
55	MG	1U	204	1/1	0.87	0.59	22,22,22,22	0
55	MG	1A	3514	1/1	0.87	0.24	38,38,38,38	0
55	MG	1a	1675	1/1	0.87	0.27	25,25,25,25	0
55	MG	10	102	1/1	0.87	0.41	36,36,36,36	0
55	MG	1A	3010	1/1	0.87	0.58	32,32,32,32	0
55	MG	2A	3541	1/1	0.87	0.21	41,41,41,41	0
55	MG	2A	3055	1/1	0.87	0.25	51,51,51,51	0
55	MG	1A	3012	1/1	0.87	0.48	15,15,15,15	0
55	MG	2A	3548	1/1	0.87	0.24	69,69,69,69	0
55	MG	2z	102	1/1	0.87	0.28	78,78,78,78	0
55	MG	1a	1826	1/1	0.87	0.22	53,53,53,53	0
55	MG	2A	3184	1/1	0.88	0.64	42,42,42,42	0
55	MG	2a	1662	1/1	0.88	0.73	90,90,90,90	0
55	MG	1a	1611	1/1	0.88	0.25	48,48,48,48	0
55	MG	1A	3230	1/1	0.88	0.61	36,36,36,36	0
55	MG	2A	3195	1/1	0.88	0.51	42,42,42,42	0
55	MG	1A	3668	1/1	0.88	0.09	43,43,43,43	0
55	MG	1a	1618	1/1	0.88	0.51	89,89,89,89	0
55	MG	1A	3534	1/1	0.88	0.14	14,14,14,14	0
55	MG	2A	3791	1/1	0.88	0.08	63,63,63,63	0
55	MG	1A	3609	1/1	0.88	0.35	63,63,63,63	0
55	MG	1A	3784	1/1	0.88	0.37	54,54,54,54	0
55	MG	1A	3109	1/1	0.88	0.09	19,19,19,19	0
55	MG	2A	3817	1/1	0.88	0.08	66,66,66,66	0
55	MG	1A	3677	1/1	0.88	0.12	57,57,57,57	0
55	MG	1A	3800	1/1	0.88	0.11	48,48,48,48	0
55	MG	2A	3829	1/1	0.88	0.26	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3094	1/1	0.88	0.84	23,23,23,23	0
55	MG	1A	3145	1/1	0.88	1.16	24,24,24,24	0
55	MG	2a	1690	1/1	0.88	0.32	53,53,53,53	0
55	MG	2F	311	1/1	0.88	0.41	72,72,72,72	0
55	MG	1d	305	1/1	0.88	0.31	59,59,59,59	0
55	MG	1A	3556	1/1	0.88	0.89	34,34,34,34	0
55	MG	2G	3003	1/1	0.88	0.11	66,66,66,66	0
55	MG	2a	1713	1/1	0.88	0.12	78,78,78,78	0
55	MG	2A	3466	1/1	0.88	0.09	37,37,37,37	0
55	MG	1A	3631	1/1	0.88	0.23	70,70,70,70	0
55	MG	1A	3847	1/1	0.88	0.13	41,41,41,41	0
55	MG	2R	201	1/1	0.88	0.95	48,48,48,48	0
55	MG	2A	3635	1/1	0.88	0.06	54,54,54,54	0
55	MG	2U	205	1/1	0.88	0.55	49,49,49,49	0
55	MG	1D	316	1/1	0.88	0.26	53,53,53,53	0
55	MG	2a	1738	1/1	0.88	0.29	83,83,83,83	0
55	MG	1a	1656	1/1	0.88	0.21	71,71,71,71	0
55	MG	1a	1766	1/1	0.88	0.10	62,62,62,62	0
55	MG	1A	3497	1/1	0.88	0.36	37,37,37,37	0
55	MG	2A	3501	1/1	0.88	0.24	41,41,41,41	0
55	MG	2A	3252	1/1	0.88	0.44	53,53,53,53	0
55	MG	2A	3126	1/1	0.88	0.26	71,71,71,71	0
55	MG	1A	3635	1/1	0.88	0.13	65,65,65,65	0
55	MG	2a	1757	1/1	0.88	0.16	69,69,69,69	0
55	MG	1A	3209	1/1	0.88	0.46	54,54,54,54	0
55	MG	1A	3871	1/1	0.88	0.40	48,48,48,48	0
55	MG	1A	3570	1/1	0.88	0.29	24,24,24,24	0
55	MG	2a	1778	1/1	0.88	0.20	63,63,63,63	0
55	MG	1A	3213	1/1	0.88	0.54	29,29,29,29	0
55	MG	2a	1782	1/1	0.88	0.16	79,79,79,79	0
55	MG	1A	3727	1/1	0.88	0.18	39,39,39,39	0
55	MG	2A	3294	1/1	0.88	0.08	77,77,77,77	0
55	MG	2a	1785	1/1	0.88	0.09	77,77,77,77	0
55	MG	2a	1793	1/1	0.88	0.58	66,66,66,66	0
55	MG	1A	3515	1/1	0.88	0.36	49,49,49,49	0
55	MG	2a	1803	1/1	0.88	0.22	81,81,81,81	0
55	MG	2A	3531	1/1	0.88	0.07	51,51,51,51	0
55	MG	13	102	1/1	0.88	1.24	32,32,32,32	0
55	MG	2A	3535	1/1	0.88	0.16	50,50,50,50	0
55	MG	2A	3539	1/1	0.88	0.12	20,20,20,20	0
55	MG	2A	3304	1/1	0.88	0.21	51,51,51,51	0
55	MG	2a	1825	1/1	0.88	0.08	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1A	3883	1/1	0.88	0.23	39,39,39,39	0
55	MG	2A	3709	1/1	0.88	0.23	78,78,78,78	0
55	MG	2A	3317	1/1	0.88	0.09	45,45,45,45	0
55	MG	2A	3319	1/1	0.88	0.23	81,81,81,81	0
55	MG	2A	3948	1/1	0.88	0.56	38,38,38,38	0
55	MG	1A	3177	1/1	0.88	0.47	46,46,46,46	0
55	MG	2a	1629	1/1	0.88	0.24	44,44,44,44	0
55	MG	2A	3168	1/1	0.88	0.79	38,38,38,38	0
55	MG	2A	3954	1/1	0.88	1.10	36,36,36,36	0
55	MG	1A	3743	1/1	0.88	0.62	19,19,19,19	0
55	MG	2A	3331	1/1	0.88	0.22	46,46,46,46	0
55	MG	1a	1801	1/1	0.88	0.19	69,69,69,69	0
55	MG	1A	3018	1/1	0.88	0.65	20,20,20,20	0
55	MG	2A	3560	1/1	0.88	0.39	85,85,85,85	0
55	MG	2A	3563	1/1	0.88	1.03	46,46,46,46	0
55	MG	2A	3566	1/1	0.88	0.27	26,26,26,26	0
55	MG	1A	3593	1/1	0.88	0.28	48,48,48,48	0
55	MG	2a	1654	1/1	0.88	0.18	42,42,42,42	0
55	MG	1A	3599	1/1	0.88	0.16	34,34,34,34	0
55	MG	1A	3657	1/1	0.88	0.52	32,32,32,32	0
56	ZN	14	501	1/1	0.88	0.03	138,138,138,138	0
55	MG	2A	3036	1/1	0.88	0.23	49,49,49,49	0
55	MG	2A	3932	1/1	0.89	0.41	56,56,56,56	0
55	MG	1A	3579	1/1	0.89	0.12	49,49,49,49	0
55	MG	1A	3648	1/1	0.89	0.13	66,66,66,66	0
55	MG	1a	1663	1/1	0.89	0.38	86,86,86,86	0
55	MG	1A	3322	1/1	0.89	0.25	30,30,30,30	0
55	MG	1G	3001	1/1	0.89	0.12	96,96,96,96	0
55	MG	2A	3683	1/1	0.89	0.14	57,57,57,57	0
55	MG	1A	3732	1/1	0.89	0.04	91,91,91,91	0
55	MG	2A	3069	1/1	0.89	0.61	36,36,36,36	0
55	MG	2A	3070	1/1	0.89	0.23	37,37,37,37	0
55	MG	2A	3958	1/1	0.89	0.21	59,59,59,59	0
55	MG	2A	3699	1/1	0.89	0.10	56,56,56,56	0
55	MG	2A	3967	1/1	0.89	0.76	48,48,48,48	0
55	MG	1A	3509	1/1	0.89	0.14	45,45,45,45	0
55	MG	2A	3970	1/1	0.89	0.49	54,54,54,54	0
55	MG	2A	3703	1/1	0.89	0.20	56,56,56,56	0
55	MG	2A	3081	1/1	0.89	0.25	40,40,40,40	0
55	MG	1A	3586	1/1	0.89	0.64	9,9,9,9	0
55	MG	2A	3258	1/1	0.89	0.73	63,63,63,63	0
55	MG	2A	3714	1/1	0.89	0.23	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	2A	3527	1/1	0.89	0.29	28,28,28,28	0
55	MG	2a	1675	1/1	0.89	0.20	44,44,44,44	0
55	MG	2A	3086	1/1	0.89	0.10	61,61,61,61	0
55	MG	1A	3077	1/1	0.89	0.24	51,51,51,51	0
55	MG	1A	3752	1/1	0.89	0.30	29,29,29,29	0
55	MG	1A	3893	1/1	0.89	0.16	53,53,53,53	0
55	MG	2A	3270	1/1	0.89	0.43	45,45,45,45	0
55	MG	10	107	1/1	0.89	0.80	40,40,40,40	0
55	MG	2A	3743	1/1	0.89	0.27	55,55,55,55	0
55	MG	11	102	1/1	0.89	0.30	36,36,36,36	0
55	MG	1A	3754	1/1	0.89	0.33	16,16,16,16	0
55	MG	1A	3656	1/1	0.89	0.96	36,36,36,36	0
55	MG	1A	3904	1/1	0.89	0.21	36,36,36,36	0
55	MG	1A	3034	1/1	0.89	0.26	18,18,18,18	0
55	MG	1a	1682	1/1	0.89	0.20	56,56,56,56	0
55	MG	2A	3316	1/1	0.89	0.22	32,32,32,32	0
55	MG	2A	3124	1/1	0.89	0.75	48,48,48,48	0
55	MG	1a	1844	1/1	0.89	0.09	70,70,70,70	0
55	MG	19	104	1/1	0.89	0.17	58,58,58,58	0
55	MG	2a	1732	1/1	0.89	0.62	78,78,78,78	0
55	MG	2D	317	1/1	0.89	0.68	61,61,61,61	0
55	MG	2A	3564	1/1	0.89	0.83	42,42,42,42	0
55	MG	1a	1686	1/1	0.89	0.24	33,33,33,33	0
55	MG	2a	1741	1/1	0.89	0.35	66,66,66,66	0
55	MG	1a	1689	1/1	0.89	0.32	59,59,59,59	0
55	MG	1a	1690	1/1	0.89	0.23	65,65,65,65	0
55	MG	1A	3038	1/1	0.89	0.79	47,47,47,47	0
55	MG	1a	1708	1/1	0.89	0.23	63,63,63,63	0
55	MG	2A	3336	1/1	0.89	0.39	57,57,57,57	0
55	MG	2A	3806	1/1	0.89	1.59	54,54,54,54	0
55	MG	1A	3453	1/1	0.89	0.08	36,36,36,36	0
55	MG	2A	3814	1/1	0.89	0.13	92,92,92,92	0
55	MG	1A	3229	1/1	0.89	0.14	42,42,42,42	0
55	MG	2R	202	1/1	0.89	0.26	43,43,43,43	0
55	MG	2a	1765	1/1	0.89	0.38	35,35,35,35	0
55	MG	2a	1766	1/1	0.89	0.09	94,94,94,94	0
55	MG	2A	3156	1/1	0.89	1.00	47,47,47,47	0
55	MG	1A	3934	1/1	0.89	0.27	67,67,67,67	0
55	MG	2A	3372	1/1	0.89	0.40	56,56,56,56	0
55	MG	2W	3002	1/1	0.89	0.31	41,41,41,41	0
55	MG	1A	3266	1/1	0.89	0.47	29,29,29,29	0
55	MG	1A	3190	1/1	0.89	0.53	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3544	1/1	0.89	0.17	51,51,51,51	0
55	MG	2a	1787	1/1	0.89	0.39	66,66,66,66	0
55	MG	2A	3395	1/1	0.89	0.11	22,22,22,22	0
55	MG	1A	3950	1/1	0.89	0.60	10,10,10,10	0
55	MG	2a	1801	1/1	0.89	0.16	86,86,86,86	0
55	MG	2A	3856	1/1	0.89	0.45	47,47,47,47	0
55	MG	1A	3195	1/1	0.89	0.19	34,34,34,34	0
55	MG	2A	3860	1/1	0.89	0.19	58,58,58,58	0
55	MG	1A	3687	1/1	0.89	0.13	46,46,46,46	0
55	MG	2A	3621	1/1	0.89	0.22	62,62,62,62	0
55	MG	1A	3197	1/1	0.89	0.24	21,21,21,21	0
55	MG	1a	1755	1/1	0.89	0.23	76,76,76,76	0
55	MG	1B	205	1/1	0.89	0.16	49,49,49,49	0
55	MG	1a	1757	1/1	0.89	0.14	83,83,83,83	0
55	MG	2a	1611	1/1	0.89	0.76	48,48,48,48	0
55	MG	1A	3140	1/1	0.89	0.93	32,32,32,32	0
55	MG	1A	3488	1/1	0.89	0.23	54,54,54,54	0
55	MG	2a	1836	1/1	0.89	0.31	46,46,46,46	0
55	MG	1A	3242	1/1	0.89	0.23	40,40,40,40	0
55	MG	2A	3457	1/1	0.89	0.28	55,55,55,55	0
55	MG	1A	3126	1/1	0.89	0.49	47,47,47,47	0
55	MG	2A	3892	1/1	0.89	0.30	61,61,61,61	0
55	MG	1a	1642	1/1	0.89	0.20	89,89,89,89	0
55	MG	1A	3104	1/1	0.89	0.79	26,26,26,26	0
55	MG	1B	228	1/1	0.89	0.16	53,53,53,53	0
55	MG	1D	303	1/1	0.89	0.73	27,27,27,27	0
55	MG	2a	1626	1/1	0.89	0.10	53,53,53,53	0
55	MG	1a	1648	1/1	0.89	0.14	44,44,44,44	0
55	MG	2a	1628	1/1	0.89	0.88	52,52,52,52	0
55	MG	2A	3482	1/1	0.89	0.40	50,50,50,50	0
55	MG	2A	3922	1/1	0.89	0.18	17,17,17,17	0
55	MG	2A	3669	1/1	0.89	0.47	31,31,31,31	0
55	MG	1a	1650	1/1	0.89	0.27	59,59,59,59	0
55	MG	1A	3575	1/1	0.89	0.18	43,43,43,43	0
55	MG	1A	3860	1/1	0.89	0.07	54,54,54,54	0
55	MG	2A	3471	1/1	0.90	0.14	61,61,61,61	0
55	MG	2A	3472	1/1	0.90	0.13	68,68,68,68	0
55	MG	2A	3651	1/1	0.90	0.21	47,47,47,47	0
55	MG	1a	1685	1/1	0.90	0.62	55,55,55,55	0
55	MG	2a	1637	1/1	0.90	0.13	47,47,47,47	0
55	MG	2A	3656	1/1	0.90	0.08	62,62,62,62	0
55	MG	1a	1621	1/1	0.90	0.24	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	1641	1/1	0.90	0.29	95,95,95,95	0
55	MG	2A	3659	1/1	0.90	1.06	45,45,45,45	0
55	MG	2A	3921	1/1	0.90	0.64	40,40,40,40	0
55	MG	2A	3663	1/1	0.90	0.16	25,25,25,25	0
55	MG	1a	1813	1/1	0.90	0.14	76,76,76,76	0
55	MG	2A	3924	1/1	0.90	0.78	43,43,43,43	0
55	MG	2A	3488	1/1	0.90	0.13	64,64,64,64	0
55	MG	2A	3243	1/1	0.90	0.85	28,28,28,28	0
55	MG	1B	219	1/1	0.90	0.09	51,51,51,51	0
55	MG	1A	3196	1/1	0.90	0.54	23,23,23,23	0
55	MG	1A	3592	1/1	0.90	0.41	23,23,23,23	0
55	MG	1A	3456	1/1	0.90	0.13	55,55,55,55	0
55	MG	1D	304	1/1	0.90	0.52	34,34,34,34	0
55	MG	2A	3507	1/1	0.90	0.17	38,38,38,38	0
55	MG	2A	3093	1/1	0.90	0.19	37,37,37,37	0
55	MG	2A	3682	1/1	0.90	0.10	49,49,49,49	0
55	MG	1a	1724	1/1	0.90	0.45	70,70,70,70	0
55	MG	1a	1730	1/1	0.90	0.35	48,48,48,48	0
55	MG	2A	3512	1/1	0.90	0.10	50,50,50,50	0
55	MG	1a	1840	1/1	0.90	0.23	81,81,81,81	0
55	MG	1a	1731	1/1	0.90	0.16	59,59,59,59	0
55	MG	2A	3108	1/1	0.90	0.85	50,50,50,50	0
55	MG	1a	1734	1/1	0.90	0.19	61,61,61,61	0
55	MG	2A	3705	1/1	0.90	0.26	54,54,54,54	0
55	MG	1A	3461	1/1	0.90	0.07	32,32,32,32	0
55	MG	1A	3749	1/1	0.90	0.16	61,61,61,61	0
55	MG	2A	3528	1/1	0.90	0.13	62,62,62,62	0
55	MG	1a	1743	1/1	0.90	0.31	58,58,58,58	0
55	MG	2a	1689	1/1	0.90	0.25	63,63,63,63	0
55	MG	2A	3298	1/1	0.90	0.11	59,59,59,59	0
55	MG	2A	3533	1/1	0.90	0.13	65,65,65,65	0
55	MG	2A	3534	1/1	0.90	0.78	43,43,43,43	0
55	MG	1A	3051	1/1	0.90	0.36	18,18,18,18	0
55	MG	2A	3729	1/1	0.90	0.12	66,66,66,66	0
55	MG	2A	3732	1/1	0.90	0.24	95,95,95,95	0
55	MG	1D	317	1/1	0.90	0.34	38,38,38,38	0
55	MG	1A	3102	1/1	0.90	0.77	39,39,39,39	0
55	MG	2A	3741	1/1	0.90	0.26	45,45,45,45	0
55	MG	1A	3149	1/1	0.90	0.41	15,15,15,15	0
55	MG	1g	3001	1/1	0.90	0.24	35,35,35,35	0
55	MG	1A	3103	1/1	0.90	0.32	29,29,29,29	0
55	MG	2A	3745	1/1	0.90	0.61	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3747	1/1	0.90	0.31	43,43,43,43	0
55	MG	2D	304	1/1	0.90	0.28	35,35,35,35	0
55	MG	2A	3749	1/1	0.90	0.38	56,56,56,56	0
55	MG	2A	3750	1/1	0.90	0.19	75,75,75,75	0
55	MG	1A	3774	1/1	0.90	0.57	54,54,54,54	0
55	MG	1A	3083	1/1	0.90	1.79	33,33,33,33	0
55	MG	1l	3002	1/1	0.90	0.25	62,62,62,62	0
55	MG	1A	3910	1/1	0.90	0.50	44,44,44,44	0
55	MG	1A	3214	1/1	0.90	0.56	22,22,22,22	0
55	MG	1a	1658	1/1	0.90	1.30	41,41,41,41	0
55	MG	2A	3766	1/1	0.90	0.05	74,74,74,74	0
55	MG	2A	3768	1/1	0.90	0.14	42,42,42,42	0
55	MG	2A	3774	1/1	0.90	0.12	49,49,49,49	0
55	MG	1V	201	1/1	0.90	0.27	16,16,16,16	0
55	MG	1A	3680	1/1	0.90	0.21	27,27,27,27	0
55	MG	2A	3342	1/1	0.90	0.20	45,45,45,45	0
55	MG	2a	1774	1/1	0.90	0.23	81,81,81,81	0
55	MG	1a	1662	1/1	0.90	0.24	72,72,72,72	0
55	MG	1A	3561	1/1	0.90	0.58	18,18,18,18	0
55	MG	1A	3257	1/1	0.90	0.77	54,54,54,54	0
55	MG	2A	3569	1/1	0.90	0.76	46,46,46,46	0
55	MG	2A	3572	1/1	0.90	0.09	67,67,67,67	0
55	MG	2U	201	1/1	0.90	0.72	55,55,55,55	0
55	MG	1A	3564	1/1	0.90	0.35	25,25,25,25	0
55	MG	2a	1788	1/1	0.90	0.18	86,86,86,86	0
55	MG	1A	3071	1/1	0.90	0.29	26,26,26,26	0
55	MG	2a	1795	1/1	0.90	0.34	53,53,53,53	0
55	MG	2A	3803	1/1	0.90	0.10	83,83,83,83	0
55	MG	2a	1799	1/1	0.90	0.15	46,46,46,46	0
55	MG	2A	3374	1/1	0.90	0.17	30,30,30,30	0
55	MG	2a	1802	1/1	0.90	0.18	95,95,95,95	0
55	MG	2A	3012	1/1	0.90	0.53	34,34,34,34	0
55	MG	2a	1804	1/1	0.90	0.07	88,88,88,88	0
55	MG	2X	102	1/1	0.90	0.20	66,66,66,66	0
55	MG	2A	3019	1/1	0.90	0.57	40,40,40,40	0
55	MG	15	102	1/1	0.90	0.37	33,33,33,33	0
55	MG	2A	3180	1/1	0.90	0.34	51,51,51,51	0
55	MG	2a	1813	1/1	0.90	0.07	72,72,72,72	0
55	MG	2A	3827	1/1	0.90	0.11	48,48,48,48	0
55	MG	2A	3397	1/1	0.90	0.49	49,49,49,49	0
55	MG	2A	3402	1/1	0.90	0.16	47,47,47,47	0
55	MG	1A	3330	1/1	0.90	0.41	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	27	102	1/1	0.90	0.11	48,48,48,48	0
55	MG	2A	3834	1/1	0.90	0.28	26,26,26,26	0
55	MG	2A	3837	1/1	0.90	0.13	42,42,42,42	0
55	MG	2A	3026	1/1	0.90	0.63	36,36,36,36	0
55	MG	1A	3716	1/1	0.90	0.34	23,23,23,23	0
55	MG	1A	3091	1/1	0.90	0.52	18,18,18,18	0
55	MG	1A	3639	1/1	0.90	0.30	33,33,33,33	0
55	MG	1A	3504	1/1	0.90	0.10	32,32,32,32	0
55	MG	1A	3840	1/1	0.90	0.28	36,36,36,36	0
55	MG	1A	3506	1/1	0.90	0.19	44,44,44,44	0
55	MG	2A	3447	1/1	0.90	0.13	29,29,29,29	0
55	MG	1A	3374	1/1	0.90	0.09	21,21,21,21	0
55	MG	2A	3037	1/1	0.90	0.25	39,39,39,39	0
55	MG	1a	1794	1/1	0.90	0.27	45,45,45,45	0
55	MG	1a	1795	1/1	0.90	0.17	66,66,66,66	0
55	MG	1B	209	1/1	0.90	0.16	41,41,41,41	0
55	MG	2A	3636	1/1	0.90	0.34	67,67,67,67	0
55	MG	1A	3120	1/1	0.90	0.26	26,26,26,26	0
55	MG	1A	3031	1/1	0.90	0.30	22,22,22,22	0
55	MG	2A	3643	1/1	0.90	1.04	49,49,49,49	0
55	MG	1A	3731	1/1	0.90	0.10	60,60,60,60	0
55	MG	1a	1717	1/1	0.91	0.19	49,49,49,49	0
55	MG	2A	3590	1/1	0.91	0.89	43,43,43,43	0
55	MG	1a	1720	1/1	0.91	0.24	79,79,79,79	0
55	MG	2A	3593	1/1	0.91	0.39	37,37,37,37	0
55	MG	2A	3831	1/1	0.91	0.20	64,64,64,64	0
55	MG	1a	1723	1/1	0.91	0.33	55,55,55,55	0
55	MG	2a	1618	1/1	0.91	0.35	96,96,96,96	0
55	MG	2A	3348	1/1	0.91	0.07	56,56,56,56	0
55	MG	1a	1610	1/1	0.91	0.55	33,33,33,33	0
55	MG	1A	3444	1/1	0.91	0.59	32,32,32,32	0
55	MG	2a	1623	1/1	0.91	0.61	41,41,41,41	0
55	MG	1A	3240	1/1	0.91	0.76	17,17,17,17	0
55	MG	1e	3001	1/1	0.91	0.15	36,36,36,36	0
55	MG	1a	1732	1/1	0.91	0.24	75,75,75,75	0
55	MG	2A	3612	1/1	0.91	0.53	65,65,65,65	0
55	MG	2A	3377	1/1	0.91	0.08	36,36,36,36	0
55	MG	1A	3143	1/1	0.91	0.20	29,29,29,29	0
55	MG	2a	1630	1/1	0.91	0.11	56,56,56,56	0
55	MG	1h	8001	1/1	0.91	0.13	64,64,64,64	0
55	MG	2A	3866	1/1	0.91	0.38	49,49,49,49	0
55	MG	2A	3392	1/1	0.91	0.22	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3393	1/1	0.91	0.10	74,74,74,74	0
55	MG	1A	3543	1/1	0.91	0.13	52,52,52,52	0
55	MG	2A	3160	1/1	0.91	0.20	41,41,41,41	0
55	MG	2A	3625	1/1	0.91	0.16	66,66,66,66	0
55	MG	2A	3396	1/1	0.91	0.17	49,49,49,49	0
55	MG	1A	3622	1/1	0.91	0.10	57,57,57,57	0
55	MG	1A	3706	1/1	0.91	0.19	20,20,20,20	0
55	MG	1A	3793	1/1	0.91	1.02	36,36,36,36	0
55	MG	1A	3243	1/1	0.91	0.19	34,34,34,34	0
55	MG	2A	3175	1/1	0.91	0.24	42,42,42,42	0
55	MG	2A	3900	1/1	0.91	0.23	69,69,69,69	0
55	MG	1A	3244	1/1	0.91	0.32	30,30,30,30	0
55	MG	2a	1659	1/1	0.91	0.41	74,74,74,74	0
55	MG	2A	3908	1/1	0.91	0.16	56,56,56,56	0
55	MG	1A	3552	1/1	0.91	0.21	12,12,12,12	0
55	MG	2A	3912	1/1	0.91	0.91	38,38,38,38	0
55	MG	2A	3642	1/1	0.91	0.21	53,53,53,53	0
55	MG	1a	1634	1/1	0.91	0.21	38,38,38,38	0
55	MG	1A	3292	1/1	0.91	0.15	40,40,40,40	0
55	MG	1A	3719	1/1	0.91	0.31	22,22,22,22	0
55	MG	2A	3649	1/1	0.91	0.17	26,26,26,26	0
55	MG	1A	3249	1/1	0.91	0.22	24,24,24,24	0
55	MG	1A	3472	1/1	0.91	0.06	28,28,28,28	0
55	MG	1A	3477	1/1	0.91	0.18	8,8,8,8	0
55	MG	2A	3191	1/1	0.91	0.44	45,45,45,45	0
55	MG	1A	3858	1/1	0.91	0.12	51,51,51,51	0
55	MG	1A	3037	1/1	0.91	0.60	30,30,30,30	0
55	MG	2A	3660	1/1	0.91	0.74	59,59,59,59	0
55	MG	2A	3937	1/1	0.91	0.18	40,40,40,40	0
55	MG	1D	307	1/1	0.91	0.78	24,24,24,24	0
55	MG	2A	3020	1/1	0.91	0.51	43,43,43,43	0
55	MG	1A	3862	1/1	0.91	0.67	42,42,42,42	0
55	MG	1A	3728	1/1	0.91	0.37	61,61,61,61	0
55	MG	1A	3317	1/1	0.91	0.18	13,13,13,13	0
55	MG	1A	3228	1/1	0.91	0.18	37,37,37,37	0
55	MG	1F	302	1/1	0.91	0.40	29,29,29,29	0
55	MG	2A	3483	1/1	0.91	0.12	36,36,36,36	0
55	MG	2a	1700	1/1	0.91	0.31	68,68,68,68	0
55	MG	1a	1773	1/1	0.91	0.28	43,43,43,43	0
55	MG	2a	1703	1/1	0.91	0.20	60,60,60,60	0
55	MG	1a	1774	1/1	0.91	0.42	66,66,66,66	0
55	MG	2A	3959	1/1	0.91	1.02	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1A	3321	1/1	0.91	0.14	17,17,17,17	0
55	MG	2A	3964	1/1	0.91	0.29	42,42,42,42	0
55	MG	2A	3491	1/1	0.91	0.21	38,38,38,38	0
55	MG	1A	3877	1/1	0.91	0.15	61,61,61,61	0
55	MG	2A	3493	1/1	0.91	0.11	53,53,53,53	0
55	MG	2a	1727	1/1	0.91	0.15	62,62,62,62	0
55	MG	2a	1728	1/1	0.91	0.20	79,79,79,79	0
55	MG	2A	3034	1/1	0.91	0.30	40,40,40,40	0
55	MG	2A	3692	1/1	0.91	0.12	46,46,46,46	0
55	MG	2A	3498	1/1	0.91	0.16	38,38,38,38	0
55	MG	1F	314	1/1	0.91	0.25	47,47,47,47	0
55	MG	2a	1739	1/1	0.91	1.65	82,82,82,82	0
55	MG	1A	3007	1/1	0.91	0.15	26,26,26,26	0
55	MG	2a	1744	1/1	0.91	0.27	72,72,72,72	0
55	MG	2A	3241	1/1	0.91	0.13	72,72,72,72	0
55	MG	1a	1782	1/1	0.91	0.38	68,68,68,68	0
55	MG	2A	3706	1/1	0.91	0.18	70,70,70,70	0
55	MG	2A	3039	1/1	0.91	0.10	45,45,45,45	0
55	MG	2A	3509	1/1	0.91	0.13	63,63,63,63	0
55	MG	1A	3135	1/1	0.91	0.28	22,22,22,22	0
55	MG	1A	3881	1/1	0.91	0.06	57,57,57,57	0
55	MG	2A	3719	1/1	0.91	0.10	25,25,25,25	0
55	MG	1A	3110	1/1	0.91	0.26	40,40,40,40	0
55	MG	2a	1761	1/1	0.91	0.12	77,77,77,77	0
55	MG	2a	1763	1/1	0.91	0.21	73,73,73,73	0
55	MG	2B	3019	1/1	0.91	0.07	63,63,63,63	0
55	MG	1U	202	1/1	0.91	0.50	27,27,27,27	0
55	MG	2B	3024	1/1	0.91	0.23	62,62,62,62	0
55	MG	2A	3052	1/1	0.91	0.70	47,47,47,47	0
55	MG	2a	1771	1/1	0.91	0.07	83,83,83,83	0
55	MG	1A	3072	1/1	0.91	0.34	37,37,37,37	0
55	MG	1A	3237	1/1	0.91	0.20	23,23,23,23	0
55	MG	2A	3731	1/1	0.91	0.23	65,65,65,65	0
55	MG	2a	1781	1/1	0.91	0.09	73,73,73,73	0
55	MG	2D	307	1/1	0.91	0.79	41,41,41,41	0
55	MG	2A	3523	1/1	0.91	0.41	38,38,38,38	0
55	MG	1a	1797	1/1	0.91	0.16	72,72,72,72	0
55	MG	2D	313	1/1	0.91	0.43	34,34,34,34	0
55	MG	1W	3002	1/1	0.91	0.24	27,27,27,27	0
55	MG	2A	3738	1/1	0.91	0.10	60,60,60,60	0
55	MG	1X	101	1/1	0.91	0.42	32,32,32,32	0
55	MG	1a	1805	1/1	0.91	0.21	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3384	1/1	0.91	0.12	46,46,46,46	0
55	MG	2A	3272	1/1	0.91	0.47	54,54,54,54	0
55	MG	2A	3273	1/1	0.91	0.47	50,50,50,50	0
55	MG	1A	3756	1/1	0.91	0.12	14,14,14,14	0
55	MG	1A	3902	1/1	0.91	0.24	55,55,55,55	0
55	MG	2A	3295	1/1	0.91	0.38	32,32,32,32	0
55	MG	1A	3903	1/1	0.91	0.19	36,36,36,36	0
55	MG	1A	3760	1/1	0.91	0.19	51,51,51,51	0
55	MG	1a	1820	1/1	0.91	0.24	65,65,65,65	0
55	MG	2A	3549	1/1	0.91	0.20	65,65,65,65	0
55	MG	2Q	203	1/1	0.91	0.90	51,51,51,51	0
55	MG	2A	3303	1/1	0.91	0.19	55,55,55,55	0
55	MG	1A	3905	1/1	0.91	0.17	61,61,61,61	0
55	MG	1A	3389	1/1	0.91	0.10	8,8,8,8	0
55	MG	1A	3911	1/1	0.91	0.19	61,61,61,61	0
55	MG	2U	203	1/1	0.91	0.17	42,42,42,42	0
55	MG	1A	3392	1/1	0.91	0.15	50,50,50,50	0
55	MG	2A	3558	1/1	0.91	0.23	15,15,15,15	0
55	MG	2a	1835	1/1	0.91	0.45	87,87,87,87	0
55	MG	2W	3001	1/1	0.91	0.19	27,27,27,27	0
55	MG	2A	3318	1/1	0.91	0.45	32,32,32,32	0
55	MG	2a	1839	1/1	0.91	0.16	62,62,62,62	0
55	MG	1A	3772	1/1	0.91	0.14	41,41,41,41	0
55	MG	2A	3562	1/1	0.91	0.70	39,39,39,39	0
55	MG	1A	3398	1/1	0.91	0.29	55,55,55,55	0
55	MG	2A	3324	1/1	0.91	0.19	28,28,28,28	0
55	MG	2A	3325	1/1	0.91	0.20	76,76,76,76	0
55	MG	2A	3788	1/1	0.91	0.11	94,94,94,94	0
55	MG	1A	3777	1/1	0.91	0.14	57,57,57,57	0
55	MG	2A	3119	1/1	0.91	0.27	35,35,35,35	0
55	MG	2l	3001	1/1	0.91	0.08	45,45,45,45	0
55	MG	2A	3799	1/1	0.91	0.60	72,72,72,72	0
55	MG	1A	3142	1/1	0.91	0.28	44,44,44,44	0
55	MG	2A	3571	1/1	0.91	0.17	50,50,50,50	0
55	MG	2A	3804	1/1	0.91	0.06	54,54,54,54	0
55	MG	1a	1711	1/1	0.91	0.19	72,72,72,72	0
55	MG	2A	3334	1/1	0.91	0.18	47,47,47,47	0
55	MG	2A	3581	1/1	0.91	0.11	55,55,55,55	0
55	MG	1A	3413	1/1	0.91	0.22	39,39,39,39	0
55	MG	1A	3872	1/1	0.92	0.45	86,86,86,86	0
55	MG	1A	3004	1/1	0.92	0.20	29,29,29,29	0
55	MG	2A	3474	1/1	0.92	0.07	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	2A	3223	1/1	0.92	0.33	48,48,48,48	0
55	MG	1F	307	1/1	0.92	0.67	25,25,25,25	0
55	MG	1A	3876	1/1	0.92	0.13	19,19,19,19	0
55	MG	2A	3889	1/1	0.92	0.14	57,57,57,57	0
55	MG	1A	3314	1/1	0.92	0.09	43,43,43,43	0
55	MG	1a	1780	1/1	0.92	0.10	45,45,45,45	0
55	MG	2A	3897	1/1	0.92	0.14	52,52,52,52	0
55	MG	1A	3070	1/1	0.92	0.47	24,24,24,24	0
55	MG	2A	3903	1/1	0.92	0.16	58,58,58,58	0
55	MG	1G	3003	1/1	0.92	0.08	43,43,43,43	0
55	MG	2A	3661	1/1	0.92	0.75	37,37,37,37	0
55	MG	1A	3457	1/1	0.92	0.14	41,41,41,41	0
55	MG	2A	3494	1/1	0.92	0.20	34,34,34,34	0
55	MG	1A	3236	1/1	0.92	0.28	22,22,22,22	0
55	MG	2A	3497	1/1	0.92	0.30	31,31,31,31	0
55	MG	2A	3048	1/1	0.92	0.50	68,68,68,68	0
55	MG	1a	1790	1/1	0.92	0.10	76,76,76,76	0
55	MG	1A	3262	1/1	0.92	0.34	44,44,44,44	0
55	MG	1A	3640	1/1	0.92	0.55	35,35,35,35	0
55	MG	1A	3039	1/1	0.92	0.11	35,35,35,35	0
55	MG	2A	3057	1/1	0.92	0.16	24,24,24,24	0
55	MG	2A	3059	1/1	0.92	0.06	67,67,67,67	0
55	MG	1A	3023	1/1	0.92	0.62	33,33,33,33	0
55	MG	2A	3064	1/1	0.92	0.19	36,36,36,36	0
55	MG	2A	3684	1/1	0.92	0.23	61,61,61,61	0
55	MG	2A	3687	1/1	0.92	0.12	80,80,80,80	0
55	MG	1A	3476	1/1	0.92	0.14	41,41,41,41	0
55	MG	1A	3901	1/1	0.92	0.12	29,29,29,29	0
55	MG	1A	3176	1/1	0.92	0.54	20,20,20,20	0
55	MG	2A	3942	1/1	0.92	0.20	30,30,30,30	0
55	MG	1Y	502	1/1	0.92	0.14	90,90,90,90	0
55	MG	2A	3698	1/1	0.92	0.07	44,44,44,44	0
55	MG	2A	3077	1/1	0.92	0.29	47,47,47,47	0
55	MG	2A	3949	1/1	0.92	1.10	37,37,37,37	0
55	MG	1A	3341	1/1	0.92	0.11	29,29,29,29	0
55	MG	10	103	1/1	0.92	0.34	45,45,45,45	0
55	MG	2A	3704	1/1	0.92	0.13	69,69,69,69	0
55	MG	2A	3955	1/1	0.92	0.25	46,46,46,46	0
55	MG	2A	3956	1/1	0.92	0.62	34,34,34,34	0
55	MG	2A	3526	1/1	0.92	0.22	60,60,60,60	0
55	MG	1A	3364	1/1	0.92	0.13	54,54,54,54	0
55	MG	1A	3568	1/1	0.92	0.08	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1A	3909	1/1	0.92	0.12	58,58,58,58	0
55	MG	2a	1699	1/1	0.92	0.12	53,53,53,53	0
55	MG	2A	3966	1/1	0.92	0.42	46,46,46,46	0
55	MG	2a	1701	1/1	0.92	0.27	84,84,84,84	0
55	MG	1a	1688	1/1	0.92	0.12	68,68,68,68	0
55	MG	2A	3713	1/1	0.92	0.25	34,34,34,34	0
55	MG	1A	3655	1/1	0.92	0.51	41,41,41,41	0
55	MG	2A	3102	1/1	0.92	0.37	45,45,45,45	0
55	MG	2A	3103	1/1	0.92	0.25	40,40,40,40	0
55	MG	2A	3538	1/1	0.92	0.21	52,52,52,52	0
55	MG	2a	1720	1/1	0.92	0.29	60,60,60,60	0
55	MG	1A	3268	1/1	0.92	0.13	32,32,32,32	0
55	MG	1A	3090	1/1	0.92	0.28	22,22,22,22	0
55	MG	1a	1834	1/1	0.92	0.33	60,60,60,60	0
55	MG	1a	1705	1/1	0.92	0.12	48,48,48,48	0
55	MG	2A	3544	1/1	0.92	0.11	29,29,29,29	0
55	MG	1A	3490	1/1	0.92	0.23	17,17,17,17	0
55	MG	2a	1734	1/1	0.92	0.15	79,79,79,79	0
55	MG	1A	3270	1/1	0.92	1.52	43,43,43,43	0
55	MG	1A	3385	1/1	0.92	0.18	47,47,47,47	0
55	MG	2A	3739	1/1	0.92	0.15	57,57,57,57	0
55	MG	2A	3740	1/1	0.92	0.26	86,86,86,86	0
55	MG	2a	1740	1/1	0.92	0.37	71,71,71,71	0
55	MG	1a	1716	1/1	0.92	0.05	71,71,71,71	0
55	MG	1A	3159	1/1	0.92	0.60	16,16,16,16	0
55	MG	2a	1746	1/1	0.92	0.10	87,87,87,87	0
55	MG	1A	3498	1/1	0.92	0.30	46,46,46,46	0
55	MG	1a	1721	1/1	0.92	0.16	49,49,49,49	0
55	MG	1A	3053	1/1	0.92	0.81	18,18,18,18	0
55	MG	2A	3746	1/1	0.92	0.29	63,63,63,63	0
55	MG	2A	3333	1/1	0.92	0.13	40,40,40,40	0
55	MG	1A	3026	1/1	0.92	0.65	22,22,22,22	0
55	MG	2A	3133	1/1	0.92	0.20	28,28,28,28	0
55	MG	2a	1756	1/1	0.92	0.12	67,67,67,67	0
55	MG	1A	3505	1/1	0.92	0.26	48,48,48,48	0
55	MG	2A	3141	1/1	0.92	0.23	35,35,35,35	0
55	MG	2A	3565	1/1	0.92	0.61	33,33,33,33	0
55	MG	2A	3761	1/1	0.92	0.15	58,58,58,58	0
55	MG	1A	3951	1/1	0.92	0.37	50,50,50,50	0
55	MG	1A	3798	1/1	0.92	0.23	60,60,60,60	0
55	MG	2A	3150	1/1	0.92	1.25	34,34,34,34	0
55	MG	2E	302	1/1	0.92	0.08	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3405	1/1	0.92	0.13	51,51,51,51	0
55	MG	1a	1736	1/1	0.92	0.16	42,42,42,42	0
55	MG	2a	1776	1/1	0.92	0.31	60,60,60,60	0
55	MG	2F	301	1/1	0.92	0.23	47,47,47,47	0
55	MG	2F	305	1/1	0.92	0.36	45,45,45,45	0
55	MG	2A	3769	1/1	0.92	0.08	62,62,62,62	0
55	MG	2A	3153	1/1	0.92	0.12	52,52,52,52	0
55	MG	1A	3058	1/1	0.92	0.08	49,49,49,49	0
55	MG	1A	3512	1/1	0.92	0.34	59,59,59,59	0
55	MG	2A	3158	1/1	0.92	0.15	37,37,37,37	0
55	MG	1a	1742	1/1	0.92	0.26	60,60,60,60	0
55	MG	1a	1627	1/1	0.92	0.10	46,46,46,46	0
55	MG	2a	1789	1/1	0.92	0.65	51,51,51,51	0
55	MG	1A	3605	1/1	0.92	0.50	44,44,44,44	0
55	MG	2Q	201	1/1	0.92	0.08	79,79,79,79	0
55	MG	2A	3592	1/1	0.92	0.82	43,43,43,43	0
55	MG	2A	3165	1/1	0.92	0.09	55,55,55,55	0
55	MG	2a	1800	1/1	0.92	0.30	68,68,68,68	0
55	MG	1A	3817	1/1	0.92	0.51	35,35,35,35	0
55	MG	2A	3794	1/1	0.92	0.13	46,46,46,46	0
55	MG	1o	101	1/1	0.92	0.28	42,42,42,42	0
55	MG	1A	3834	1/1	0.92	0.06	60,60,60,60	0
55	MG	1A	3607	1/1	0.92	0.14	16,16,16,16	0
55	MG	1A	3078	1/1	0.92	0.88	30,30,30,30	0
55	MG	2A	3405	1/1	0.92	0.17	51,51,51,51	0
55	MG	2A	3406	1/1	0.92	0.19	45,45,45,45	0
55	MG	2A	3611	1/1	0.92	0.24	47,47,47,47	0
55	MG	1A	3612	1/1	0.92	0.10	50,50,50,50	0
55	MG	2A	3815	1/1	0.92	0.20	47,47,47,47	0
55	MG	2A	3613	1/1	0.92	0.12	33,33,33,33	0
55	MG	2A	3818	1/1	0.92	0.19	50,50,50,50	0
55	MG	2a	1829	1/1	0.92	0.12	64,64,64,64	0
55	MG	2A	3415	1/1	0.92	0.32	46,46,46,46	0
55	MG	1a	1636	1/1	0.92	0.31	62,62,62,62	0
55	MG	1B	226	1/1	0.92	0.07	49,49,49,49	0
55	MG	1A	3435	1/1	0.92	0.06	47,47,47,47	0
55	MG	1A	3857	1/1	0.92	0.21	52,52,52,52	0
55	MG	1A	3615	1/1	0.92	0.20	52,52,52,52	0
55	MG	1A	3443	1/1	0.92	0.07	45,45,45,45	0
55	MG	2A	3013	1/1	0.92	0.21	31,31,31,31	0
55	MG	2b	3001	1/1	0.92	0.13	68,68,68,68	0
55	MG	1A	3617	1/1	0.92	0.16	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3863	1/1	0.92	0.18	66,66,66,66	0
55	MG	1D	312	1/1	0.92	0.29	24,24,24,24	0
55	MG	2A	3458	1/1	0.92	0.10	46,46,46,46	0
55	MG	2A	3634	1/1	0.92	0.06	68,68,68,68	0
55	MG	1a	1768	1/1	0.92	0.19	75,75,75,75	0
55	MG	2a	1614	1/1	0.92	0.15	32,32,32,32	0
55	MG	2A	3858	1/1	0.92	0.50	51,51,51,51	0
55	MG	1A	3519	1/1	0.92	0.32	27,27,27,27	0
55	MG	2A	3639	1/1	0.92	0.27	36,36,36,36	0
55	MG	2o	102	1/1	0.92	0.20	38,38,38,38	0
55	MG	2A	3862	1/1	0.92	0.08	63,63,63,63	0
55	MG	2A	3865	1/1	0.92	0.11	56,56,56,56	0
55	MG	1a	1655	1/1	0.92	0.16	35,35,35,35	0
55	MG	2A	3205	1/1	0.92	0.67	42,42,42,42	0
55	MG	1A	3301	1/1	0.92	0.11	32,32,32,32	0
55	MG	1A	3451	1/1	0.92	0.26	48,48,48,48	0
55	MG	2A	3629	1/1	0.93	0.29	48,48,48,48	0
55	MG	2A	3410	1/1	0.93	0.08	54,54,54,54	0
55	MG	1a	1619	1/1	0.93	0.17	52,52,52,52	0
55	MG	1a	1620	1/1	0.93	0.14	77,77,77,77	0
55	MG	2A	3171	1/1	0.93	0.25	40,40,40,40	0
55	MG	2A	3173	1/1	0.93	0.12	69,69,69,69	0
55	MG	2A	3870	1/1	0.93	0.26	48,48,48,48	0
55	MG	2A	3871	1/1	0.93	0.63	39,39,39,39	0
55	MG	1A	3751	1/1	0.93	0.51	21,21,21,21	0
55	MG	2A	3423	1/1	0.93	0.11	49,49,49,49	0
55	MG	2A	3432	1/1	0.93	0.11	38,38,38,38	0
55	MG	2A	3880	1/1	0.93	0.10	58,58,58,58	0
55	MG	1B	224	1/1	0.93	0.14	63,63,63,63	0
55	MG	2A	3882	1/1	0.93	0.72	64,64,64,64	0
55	MG	1A	3867	1/1	0.93	0.31	48,48,48,48	0
55	MG	2A	3440	1/1	0.93	0.25	27,27,27,27	0
55	MG	1A	3658	1/1	0.93	0.08	27,27,27,27	0
55	MG	1a	1749	1/1	0.93	0.22	68,68,68,68	0
55	MG	2a	1642	1/1	0.93	0.33	80,80,80,80	0
55	MG	2A	3449	1/1	0.93	0.10	50,50,50,50	0
55	MG	2a	1645	1/1	0.93	0.45	33,33,33,33	0
55	MG	1A	3445	1/1	0.93	0.24	19,19,19,19	0
55	MG	2A	3893	1/1	0.93	1.02	55,55,55,55	0
55	MG	2A	3894	1/1	0.93	0.31	38,38,38,38	0
55	MG	1A	3020	1/1	0.93	0.36	22,22,22,22	0
55	MG	2A	3181	1/1	0.93	0.63	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	1752	1/1	0.93	0.21	86,86,86,86	0
55	MG	1A	3610	1/1	0.93	0.70	30,30,30,30	0
55	MG	1A	3761	1/1	0.93	0.45	30,30,30,30	0
55	MG	2A	3188	1/1	0.93	0.33	39,39,39,39	0
55	MG	1D	309	1/1	0.93	0.43	27,27,27,27	0
55	MG	2A	3913	1/1	0.93	0.14	55,55,55,55	0
55	MG	2A	3664	1/1	0.93	0.21	51,51,51,51	0
55	MG	2A	3192	1/1	0.93	0.86	44,44,44,44	0
55	MG	1A	3671	1/1	0.93	0.13	42,42,42,42	0
55	MG	1A	3137	1/1	0.93	0.22	33,33,33,33	0
55	MG	2A	3920	1/1	0.93	0.52	54,54,54,54	0
55	MG	1D	314	1/1	0.93	0.29	42,42,42,42	0
55	MG	1A	3766	1/1	0.93	0.17	24,24,24,24	0
55	MG	1a	1760	1/1	0.93	0.16	76,76,76,76	0
55	MG	1A	3558	1/1	0.93	0.82	19,19,19,19	0
55	MG	2A	3484	1/1	0.93	0.12	25,25,25,25	0
55	MG	2A	3203	1/1	0.93	0.20	36,36,36,36	0
55	MG	1A	3191	1/1	0.93	0.45	31,31,31,31	0
55	MG	2A	3681	1/1	0.93	0.26	82,82,82,82	0
55	MG	1a	1646	1/1	0.93	0.59	47,47,47,47	0
55	MG	2a	1682	1/1	0.93	0.46	73,73,73,73	0
55	MG	1E	302	1/1	0.93	0.63	18,18,18,18	0
55	MG	2a	1685	1/1	0.93	0.09	47,47,47,47	0
55	MG	1E	305	1/1	0.93	0.14	25,25,25,25	0
55	MG	2A	3685	1/1	0.93	0.15	56,56,56,56	0
55	MG	1A	3888	1/1	0.93	0.13	60,60,60,60	0
55	MG	2A	3221	1/1	0.93	0.33	30,30,30,30	0
55	MG	1a	1652	1/1	0.93	0.40	41,41,41,41	0
55	MG	1A	3890	1/1	0.93	0.21	21,21,21,21	0
55	MG	1A	3380	1/1	0.93	0.10	23,23,23,23	0
55	MG	2A	3696	1/1	0.93	0.13	48,48,48,48	0
55	MG	1A	3015	1/1	0.93	0.52	33,33,33,33	0
55	MG	1a	1776	1/1	0.93	0.07	66,66,66,66	0
55	MG	2a	1705	1/1	0.93	0.76	63,63,63,63	0
55	MG	2a	1706	1/1	0.93	0.11	58,58,58,58	0
55	MG	2A	3503	1/1	0.93	0.23	62,62,62,62	0
55	MG	2A	3702	1/1	0.93	0.37	50,50,50,50	0
55	MG	2a	1714	1/1	0.93	0.21	55,55,55,55	0
55	MG	2A	3042	1/1	0.93	0.46	29,29,29,29	0
55	MG	2a	1718	1/1	0.93	0.11	38,38,38,38	0
55	MG	1F	310	1/1	0.93	0.12	18,18,18,18	0
55	MG	2A	3047	1/1	0.93	0.19	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1F	313	1/1	0.93	0.20	4,4,4,4	0
55	MG	1a	1660	1/1	0.93	0.31	57,57,57,57	0
55	MG	2A	3246	1/1	0.93	0.36	56,56,56,56	0
55	MG	2A	3247	1/1	0.93	0.53	48,48,48,48	0
55	MG	2A	3050	1/1	0.93	0.88	48,48,48,48	0
55	MG	1A	3459	1/1	0.93	0.14	8,8,8,8	0
55	MG	2A	3717	1/1	0.93	0.20	43,43,43,43	0
55	MG	2A	3718	1/1	0.93	0.20	44,44,44,44	0
55	MG	1A	3106	1/1	0.93	0.28	27,27,27,27	0
55	MG	1a	1783	1/1	0.93	0.09	60,60,60,60	0
55	MG	1G	3002	1/1	0.93	0.08	49,49,49,49	0
55	MG	2A	3723	1/1	0.93	0.55	65,65,65,65	0
55	MG	1A	3692	1/1	0.93	0.14	29,29,29,29	0
55	MG	2A	3525	1/1	0.93	0.35	33,33,33,33	0
55	MG	2a	1745	1/1	0.93	0.09	70,70,70,70	0
55	MG	1H	202	1/1	0.93	0.14	51,51,51,51	0
55	MG	2A	3062	1/1	0.93	0.34	40,40,40,40	0
55	MG	1A	3036	1/1	0.93	0.10	56,56,56,56	0
55	MG	2A	3733	1/1	0.93	0.25	62,62,62,62	0
55	MG	2A	3065	1/1	0.93	0.17	12,12,12,12	0
55	MG	2A	3268	1/1	0.93	0.22	55,55,55,55	0
55	MG	2a	1753	1/1	0.93	0.23	102,102,102,102	0
55	MG	2A	3066	1/1	0.93	0.77	46,46,46,46	0
55	MG	1A	3626	1/1	0.93	0.12	68,68,68,68	0
55	MG	1a	1792	1/1	0.93	0.24	60,60,60,60	0
55	MG	1R	203	1/1	0.93	0.21	31,31,31,31	0
55	MG	1A	3709	1/1	0.93	0.10	31,31,31,31	0
55	MG	2A	3280	1/1	0.93	0.10	33,33,33,33	0
55	MG	2a	1762	1/1	0.93	0.13	71,71,71,71	0
55	MG	1A	3713	1/1	0.93	0.20	22,22,22,22	0
55	MG	1A	3513	1/1	0.93	0.16	46,46,46,46	0
55	MG	2D	311	1/1	0.93	0.39	24,24,24,24	0
55	MG	1U	205	1/1	0.93	0.31	22,22,22,22	0
55	MG	1a	1804	1/1	0.93	0.15	52,52,52,52	0
55	MG	2A	3087	1/1	0.93	0.46	43,43,43,43	0
55	MG	2a	1772	1/1	0.93	0.07	57,57,57,57	0
55	MG	2A	3550	1/1	0.93	0.14	53,53,53,53	0
55	MG	2a	1775	1/1	0.93	0.07	54,54,54,54	0
55	MG	2A	3091	1/1	0.93	0.79	38,38,38,38	0
55	MG	1A	3252	1/1	0.93	2.05	41,41,41,41	0
55	MG	2A	3308	1/1	0.93	0.15	36,36,36,36	0
55	MG	2a	1780	1/1	0.93	0.14	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3129	1/1	0.93	0.20	17,17,17,17	0
55	MG	1A	3475	1/1	0.93	0.34	37,37,37,37	0
55	MG	1A	3064	1/1	0.93	0.22	20,20,20,20	0
55	MG	1A	3585	1/1	0.93	0.20	29,29,29,29	0
55	MG	1A	3920	1/1	0.93	0.75	33,33,33,33	0
55	MG	2a	1786	1/1	0.93	0.30	52,52,52,52	0
55	MG	1A	3814	1/1	0.93	0.16	41,41,41,41	0
55	MG	2A	3322	1/1	0.93	0.10	62,62,62,62	0
55	MG	2A	3773	1/1	0.93	0.10	46,46,46,46	0
55	MG	2a	1790	1/1	0.93	0.11	57,57,57,57	0
55	MG	1A	3815	1/1	0.93	0.06	57,57,57,57	0
55	MG	2a	1794	1/1	0.93	0.04	92,92,92,92	0
55	MG	1A	3005	1/1	0.93	0.18	20,20,20,20	0
55	MG	2H	8002	1/1	0.93	1.36	90,90,90,90	0
55	MG	1A	3945	1/1	0.93	0.24	22,22,22,22	0
55	MG	2N	203	1/1	0.93	0.50	90,90,90,90	0
55	MG	2P	201	1/1	0.93	0.62	31,31,31,31	0
55	MG	1A	3826	1/1	0.93	0.07	60,60,60,60	0
55	MG	2A	3114	1/1	0.93	0.16	43,43,43,43	0
55	MG	15	106	1/1	0.93	0.11	50,50,50,50	0
55	MG	2A	3118	1/1	0.93	0.30	44,44,44,44	0
55	MG	1a	1691	1/1	0.93	0.21	59,59,59,59	0
55	MG	1a	1836	1/1	0.93	0.13	53,53,53,53	0
55	MG	1a	1697	1/1	0.93	0.12	53,53,53,53	0
55	MG	2a	1812	1/1	0.93	0.11	69,69,69,69	0
55	MG	2U	202	1/1	0.93	0.78	39,39,39,39	0
55	MG	1a	1702	1/1	0.93	0.08	46,46,46,46	0
55	MG	2A	3344	1/1	0.93	0.12	49,49,49,49	0
55	MG	2A	3587	1/1	0.93	0.19	38,38,38,38	0
55	MG	1A	3947	1/1	0.93	0.55	24,24,24,24	0
55	MG	1A	3275	1/1	0.93	0.16	11,11,11,11	0
55	MG	1a	1843	1/1	0.93	0.23	57,57,57,57	0
55	MG	18	3302	1/1	0.93	0.77	24,24,24,24	0
55	MG	1A	3591	1/1	0.93	0.32	60,60,60,60	0
55	MG	1A	3956	1/1	0.93	0.54	21,21,21,21	0
55	MG	1A	3419	1/1	0.93	0.22	39,39,39,39	0
55	MG	2A	3376	1/1	0.93	0.12	58,58,58,58	0
55	MG	1A	3434	1/1	0.93	0.13	20,20,20,20	0
55	MG	2a	1840	1/1	0.93	0.09	59,59,59,59	0
55	MG	2A	3149	1/1	0.93	1.04	43,43,43,43	0
55	MG	2A	3823	1/1	0.93	0.06	60,60,60,60	0
55	MG	2A	3825	1/1	0.93	0.12	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1a	1603	1/1	0.93	0.23	49,49,49,49	0
55	MG	2A	3384	1/1	0.93	0.17	35,35,35,35	0
55	MG	2A	3388	1/1	0.93	0.21	56,56,56,56	0
55	MG	2a	1603	1/1	0.93	0.09	93,93,93,93	0
55	MG	2A	3390	1/1	0.93	0.19	41,41,41,41	0
55	MG	1A	3596	1/1	0.93	0.13	46,46,46,46	0
55	MG	2A	3617	1/1	0.93	0.13	59,59,59,59	0
55	MG	1A	3598	1/1	0.93	0.22	61,61,61,61	0
55	MG	1A	3539	1/1	0.93	0.08	17,17,17,17	0
55	MG	1A	3739	1/1	0.93	0.09	49,49,49,49	0
55	MG	1a	1612	1/1	0.93	0.20	60,60,60,60	0
55	MG	1a	1613	1/1	0.93	0.15	26,26,26,26	0
55	MG	1A	3335	1/1	0.93	0.40	36,36,36,36	0
55	MG	1A	3164	1/1	0.93	0.30	23,23,23,23	0
55	MG	1a	1739	1/1	0.93	0.18	67,67,67,67	0
55	MG	1A	3358	1/1	0.93	0.10	33,33,33,33	0
55	MG	1A	3069	1/1	0.94	0.48	17,17,17,17	0
55	MG	1A	3367	1/1	0.94	0.11	24,24,24,24	0
55	MG	2A	3477	1/1	0.94	0.29	32,32,32,32	0
55	MG	2A	3730	1/1	0.94	0.35	43,43,43,43	0
55	MG	1a	1831	1/1	0.94	0.33	66,66,66,66	0
55	MG	1a	1649	1/1	0.94	0.28	47,47,47,47	0
55	MG	1A	3368	1/1	0.94	0.13	13,13,13,13	0
55	MG	1a	1651	1/1	0.94	0.16	43,43,43,43	0
55	MG	1A	3371	1/1	0.94	0.06	17,17,17,17	0
55	MG	1A	3099	1/1	0.94	0.32	29,29,29,29	0
55	MG	1A	3503	1/1	0.94	0.10	60,60,60,60	0
55	MG	1A	3154	1/1	0.94	0.83	41,41,41,41	0
55	MG	1A	3201	1/1	0.94	0.24	29,29,29,29	0
55	MG	1A	3383	1/1	0.94	0.20	13,13,13,13	0
55	MG	2A	3186	1/1	0.94	0.84	50,50,50,50	0
55	MG	2V	203	1/1	0.94	0.52	58,58,58,58	0
55	MG	1A	3156	1/1	0.94	0.21	20,20,20,20	0
55	MG	1A	3770	1/1	0.94	0.06	45,45,45,45	0
55	MG	1B	220	1/1	0.94	0.06	29,29,29,29	0
55	MG	1A	3511	1/1	0.94	0.22	46,46,46,46	0
55	MG	2A	3193	1/1	0.94	0.32	45,45,45,45	0
55	MG	1B	225	1/1	0.94	0.19	36,36,36,36	0
55	MG	2A	3506	1/1	0.94	0.13	55,55,55,55	0
55	MG	1a	1667	1/1	0.94	0.41	63,63,63,63	0
55	MG	2A	3197	1/1	0.94	0.17	52,52,52,52	0
55	MG	2A	3756	1/1	0.94	0.55	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3757	1/1	0.94	0.23	60,60,60,60	0
55	MG	2A	3198	1/1	0.94	0.25	49,49,49,49	0
55	MG	25	102	1/1	0.94	0.25	41,41,41,41	0
55	MG	1A	3128	1/1	0.94	0.20	22,22,22,22	0
55	MG	1A	3267	1/1	0.94	0.18	20,20,20,20	0
55	MG	28	102	1/1	0.94	0.08	60,60,60,60	0
55	MG	1A	3390	1/1	0.94	0.11	36,36,36,36	0
55	MG	1D	301	1/1	0.94	0.18	21,21,21,21	0
55	MG	2a	1602	1/1	0.94	0.13	60,60,60,60	0
55	MG	1A	3030	1/1	0.94	0.26	10,10,10,10	0
55	MG	2A	3204	1/1	0.94	0.49	31,31,31,31	0
55	MG	1A	3397	1/1	0.94	0.19	77,77,77,77	0
55	MG	2A	3522	1/1	0.94	0.14	32,32,32,32	0
55	MG	2a	1610	1/1	0.94	0.20	79,79,79,79	0
55	MG	1D	306	1/1	0.94	0.12	17,17,17,17	0
55	MG	1A	3162	1/1	0.94	0.15	45,45,45,45	0
55	MG	1A	3520	1/1	0.94	0.15	35,35,35,35	0
55	MG	2A	3213	1/1	0.94	0.54	37,37,37,37	0
55	MG	2A	3214	1/1	0.94	0.58	32,32,32,32	0
55	MG	1A	3521	1/1	0.94	0.31	19,19,19,19	0
55	MG	1A	3522	1/1	0.94	0.14	71,71,71,71	0
55	MG	1A	3221	1/1	0.94	0.40	34,34,34,34	0
55	MG	2A	3789	1/1	0.94	0.11	41,41,41,41	0
55	MG	2A	3225	1/1	0.94	0.18	30,30,30,30	0
55	MG	1A	3059	1/1	0.94	0.12	51,51,51,51	0
55	MG	1A	3082	1/1	0.94	0.96	32,32,32,32	0
55	MG	2A	3537	1/1	0.94	0.21	65,65,65,65	0
55	MG	1A	3799	1/1	0.94	0.09	35,35,35,35	0
55	MG	1A	3536	1/1	0.94	0.15	40,40,40,40	0
55	MG	1A	3537	1/1	0.94	0.43	54,54,54,54	0
55	MG	1F	301	1/1	0.94	0.21	17,17,17,17	0
55	MG	1A	3415	1/1	0.94	0.07	49,49,49,49	0
55	MG	2A	3812	1/1	0.94	0.06	53,53,53,53	0
55	MG	1A	3047	1/1	0.94	0.14	31,31,31,31	0
55	MG	2a	1632	1/1	0.94	0.08	55,55,55,55	0
55	MG	1F	306	1/1	0.94	0.53	26,26,26,26	0
55	MG	1a	1694	1/1	0.94	0.32	48,48,48,48	0
55	MG	1A	3426	1/1	0.94	0.10	15,15,15,15	0
55	MG	2A	3017	1/1	0.94	0.66	36,36,36,36	0
55	MG	2A	3820	1/1	0.94	0.10	36,36,36,36	0
55	MG	2A	3249	1/1	0.94	0.14	67,67,67,67	0
55	MG	1A	3280	1/1	0.94	0.14	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1A	3548	1/1	0.94	0.12	27,27,27,27	0
55	MG	1A	3823	1/1	0.94	0.09	60,60,60,60	0
55	MG	2A	3254	1/1	0.94	0.49	74,74,74,74	0
55	MG	2A	3830	1/1	0.94	0.12	71,71,71,71	0
55	MG	2a	1647	1/1	0.94	0.27	67,67,67,67	0
55	MG	2A	3255	1/1	0.94	0.22	35,35,35,35	0
55	MG	2A	3832	1/1	0.94	0.98	39,39,39,39	0
55	MG	1a	1706	1/1	0.94	0.20	44,44,44,44	0
55	MG	2A	3561	1/1	0.94	0.58	55,55,55,55	0
55	MG	2a	1657	1/1	0.94	0.67	46,46,46,46	0
55	MG	2A	3836	1/1	0.94	0.13	79,79,79,79	0
55	MG	1A	3285	1/1	0.94	0.20	12,12,12,12	0
55	MG	2A	3839	1/1	0.94	0.09	28,28,28,28	0
55	MG	1A	3663	1/1	0.94	0.12	77,77,77,77	0
55	MG	2A	3843	1/1	0.94	0.10	38,38,38,38	0
55	MG	1a	1713	1/1	0.94	0.15	36,36,36,36	0
55	MG	2A	3847	1/1	0.94	0.12	52,52,52,52	0
55	MG	1a	1714	1/1	0.94	0.06	49,49,49,49	0
55	MG	1A	3664	1/1	0.94	0.21	31,31,31,31	0
55	MG	2A	3854	1/1	0.94	0.18	35,35,35,35	0
55	MG	1A	3843	1/1	0.94	0.91	25,25,25,25	0
55	MG	2A	3269	1/1	0.94	0.39	51,51,51,51	0
55	MG	1A	3665	1/1	0.94	0.43	23,23,23,23	0
55	MG	2A	3570	1/1	0.94	0.51	53,53,53,53	0
55	MG	1A	3551	1/1	0.94	0.21	47,47,47,47	0
55	MG	1A	3848	1/1	0.94	0.17	63,63,63,63	0
55	MG	2A	3864	1/1	0.94	0.42	47,47,47,47	0
55	MG	2A	3576	1/1	0.94	0.22	25,25,25,25	0
55	MG	1A	3853	1/1	0.94	0.07	47,47,47,47	0
55	MG	2a	1679	1/1	0.94	0.67	27,27,27,27	0
55	MG	2a	1680	1/1	0.94	0.13	82,82,82,82	0
55	MG	2A	3274	1/1	0.94	1.04	51,51,51,51	0
55	MG	2A	3277	1/1	0.94	0.46	39,39,39,39	0
55	MG	2a	1683	1/1	0.94	0.76	48,48,48,48	0
55	MG	2A	3869	1/1	0.94	0.09	50,50,50,50	0
55	MG	1A	3436	1/1	0.94	0.15	11,11,11,11	0
55	MG	1A	3288	1/1	0.94	0.38	7,7,7,7	0
55	MG	2a	1688	1/1	0.94	0.29	71,71,71,71	0
55	MG	2A	3589	1/1	0.94	0.47	43,43,43,43	0
55	MG	2A	3873	1/1	0.94	0.16	80,80,80,80	0
55	MG	2A	3284	1/1	0.94	0.08	79,79,79,79	0
55	MG	2A	3286	1/1	0.94	0.13	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3876	1/1	0.94	0.27	38,38,38,38	0
55	MG	1A	3169	1/1	0.94	0.28	46,46,46,46	0
55	MG	1A	3557	1/1	0.94	0.95	32,32,32,32	0
55	MG	1A	3108	1/1	0.94	0.94	24,24,24,24	0
55	MG	2A	3883	1/1	0.94	0.23	71,71,71,71	0
55	MG	1V	202	1/1	0.94	0.44	19,19,19,19	0
55	MG	1W	3001	1/1	0.94	0.20	14,14,14,14	0
55	MG	1A	3678	1/1	0.94	0.10	32,32,32,32	0
55	MG	1W	3003	1/1	0.94	0.33	21,21,21,21	0
55	MG	1A	3679	1/1	0.94	0.17	36,36,36,36	0
55	MG	2A	3606	1/1	0.94	0.71	66,66,66,66	0
55	MG	1A	3865	1/1	0.94	0.14	48,48,48,48	0
55	MG	1A	3560	1/1	0.94	0.21	34,34,34,34	0
55	MG	1a	1745	1/1	0.94	0.28	61,61,61,61	0
55	MG	1A	3446	1/1	0.94	0.07	76,76,76,76	0
55	MG	2A	3901	1/1	0.94	0.35	54,54,54,54	0
55	MG	2a	1723	1/1	0.94	0.07	73,73,73,73	0
55	MG	1A	3686	1/1	0.94	0.10	22,22,22,22	0
55	MG	2a	1726	1/1	0.94	0.51	46,46,46,46	0
55	MG	2A	3906	1/1	0.94	0.28	79,79,79,79	0
55	MG	10	104	1/1	0.94	0.07	34,34,34,34	0
55	MG	2a	1730	1/1	0.94	0.16	81,81,81,81	0
55	MG	1A	3294	1/1	0.94	0.13	22,22,22,22	0
55	MG	2A	3909	1/1	0.94	0.06	58,58,58,58	0
55	MG	1A	3563	1/1	0.94	0.47	28,28,28,28	0
55	MG	11	104	1/1	0.94	0.18	24,24,24,24	0
55	MG	1A	3063	1/1	0.94	0.19	41,41,41,41	0
55	MG	15	101	1/1	0.94	0.76	19,19,19,19	0
55	MG	1A	3695	1/1	0.94	0.13	50,50,50,50	0
55	MG	2A	3071	1/1	0.94	0.27	43,43,43,43	0
55	MG	2A	3918	1/1	0.94	0.26	70,70,70,70	0
55	MG	15	103	1/1	0.94	0.18	19,19,19,19	0
55	MG	2A	3074	1/1	0.94	0.44	46,46,46,46	0
55	MG	1A	3698	1/1	0.94	0.12	25,25,25,25	0
55	MG	1A	3139	1/1	0.94	0.36	33,33,33,33	0
55	MG	1A	3700	1/1	0.94	0.11	48,48,48,48	0
55	MG	2A	3343	1/1	0.94	0.15	39,39,39,39	0
55	MG	2A	3925	1/1	0.94	0.50	24,24,24,24	0
55	MG	1A	3702	1/1	0.94	0.14	43,43,43,43	0
55	MG	18	3303	1/1	0.94	0.07	56,56,56,56	0
55	MG	2A	3638	1/1	0.94	0.07	51,51,51,51	0
55	MG	1A	3055	1/1	0.94	0.24	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	2A	3933	1/1	0.94	0.19	36,36,36,36	0
55	MG	2A	3935	1/1	0.94	0.44	49,49,49,49	0
55	MG	2A	3936	1/1	0.94	0.21	35,35,35,35	0
55	MG	2A	3092	1/1	0.94	0.38	47,47,47,47	0
55	MG	2A	3356	1/1	0.94	0.14	29,29,29,29	0
55	MG	1A	3141	1/1	0.94	0.12	36,36,36,36	0
55	MG	2A	3365	1/1	0.94	0.18	72,72,72,72	0
55	MG	1A	3710	1/1	0.94	0.15	36,36,36,36	0
55	MG	2A	3645	1/1	0.94	0.28	33,33,33,33	0
55	MG	2a	1769	1/1	0.94	0.40	83,83,83,83	0
55	MG	2a	1770	1/1	0.94	0.13	72,72,72,72	0
55	MG	1a	1769	1/1	0.94	0.27	62,62,62,62	0
55	MG	1A	3891	1/1	0.94	0.21	34,34,34,34	0
55	MG	2a	1773	1/1	0.94	0.18	84,84,84,84	0
55	MG	2A	3101	1/1	0.94	0.45	36,36,36,36	0
55	MG	1A	3112	1/1	0.94	0.35	46,46,46,46	0
55	MG	2A	3652	1/1	0.94	0.15	40,40,40,40	0
55	MG	1A	3115	1/1	0.94	0.14	23,23,23,23	0
55	MG	1A	3464	1/1	0.94	0.12	38,38,38,38	0
55	MG	2A	3381	1/1	0.94	0.34	47,47,47,47	0
55	MG	2A	3957	1/1	0.94	0.11	61,61,61,61	0
55	MG	1A	3118	1/1	0.94	0.09	35,35,35,35	0
55	MG	1A	3583	1/1	0.94	0.16	21,21,21,21	0
55	MG	2A	3389	1/1	0.94	0.18	25,25,25,25	0
55	MG	2A	3962	1/1	0.94	0.33	32,32,32,32	0
55	MG	2A	3963	1/1	0.94	0.18	64,64,64,64	0
55	MG	1A	3075	1/1	0.94	0.57	21,21,21,21	0
55	MG	2A	3965	1/1	0.94	0.51	42,42,42,42	0
55	MG	1A	3720	1/1	0.94	0.14	40,40,40,40	0
55	MG	2A	3113	1/1	0.94	0.17	35,35,35,35	0
55	MG	2a	1791	1/1	0.94	0.09	47,47,47,47	0
55	MG	2A	3968	1/1	0.94	1.08	34,34,34,34	0
55	MG	2A	3668	1/1	0.94	0.34	44,44,44,44	0
55	MG	1A	3188	1/1	0.94	0.24	33,33,33,33	0
55	MG	1A	3328	1/1	0.94	0.12	45,45,45,45	0
55	MG	2a	1798	1/1	0.94	0.11	46,46,46,46	0
55	MG	1a	1616	1/1	0.94	0.54	75,75,75,75	0
55	MG	1A	3329	1/1	0.94	0.08	67,67,67,67	0
55	MG	2A	3674	1/1	0.94	0.24	55,55,55,55	0
55	MG	1A	3725	1/1	0.94	0.19	29,29,29,29	0
55	MG	2A	3403	1/1	0.94	0.11	68,68,68,68	0
55	MG	2A	3121	1/1	0.94	0.16	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	1805	1/1	0.94	0.30	66,66,66,66	0
55	MG	2A	3122	1/1	0.94	0.07	44,44,44,44	0
55	MG	1A	3092	1/1	0.94	0.21	11,11,11,11	0
55	MG	2B	3013	1/1	0.94	0.07	66,66,66,66	0
55	MG	1A	3065	1/1	0.94	0.35	11,11,11,11	0
55	MG	1a	1623	1/1	0.94	0.13	63,63,63,63	0
55	MG	1a	1624	1/1	0.94	0.44	49,49,49,49	0
55	MG	2a	1814	1/1	0.94	0.05	66,66,66,66	0
55	MG	2A	3131	1/1	0.94	0.14	44,44,44,44	0
55	MG	1A	3125	1/1	0.94	0.76	26,26,26,26	0
55	MG	1A	3482	1/1	0.94	0.18	37,37,37,37	0
55	MG	1A	3484	1/1	0.94	0.18	38,38,38,38	0
55	MG	2A	3425	1/1	0.94	0.07	32,32,32,32	0
55	MG	2A	3691	1/1	0.94	0.10	49,49,49,49	0
55	MG	1A	3921	1/1	0.94	0.19	35,35,35,35	0
55	MG	1a	1796	1/1	0.94	0.17	57,57,57,57	0
55	MG	2A	3437	1/1	0.94	0.10	44,44,44,44	0
55	MG	2A	3145	1/1	0.94	0.12	42,42,42,42	0
55	MG	1A	3923	1/1	0.94	0.11	26,26,26,26	0
55	MG	2D	309	1/1	0.94	0.70	47,47,47,47	0
55	MG	1A	3929	1/1	0.94	0.18	25,25,25,25	0
55	MG	2A	3444	1/1	0.94	0.11	36,36,36,36	0
55	MG	1A	3344	1/1	0.94	0.10	21,21,21,21	0
55	MG	2A	3448	1/1	0.94	0.09	41,41,41,41	0
55	MG	2d	503	1/1	0.94	0.34	77,77,77,77	0
55	MG	1a	1802	1/1	0.94	0.07	67,67,67,67	0
55	MG	1A	3734	1/1	0.94	0.07	26,26,26,26	0
55	MG	2A	3454	1/1	0.94	0.12	38,38,38,38	0
55	MG	2E	301	1/1	0.94	0.18	63,63,63,63	0
55	MG	1A	3349	1/1	0.94	0.12	31,31,31,31	0
55	MG	2E	303	1/1	0.94	1.14	37,37,37,37	0
55	MG	1A	3742	1/1	0.94	0.07	77,77,77,77	0
55	MG	1A	3489	1/1	0.94	0.14	23,23,23,23	0
55	MG	1a	1808	1/1	0.94	0.18	67,67,67,67	0
55	MG	1A	3150	1/1	0.94	0.12	41,41,41,41	0
55	MG	2F	309	1/1	0.94	0.74	42,42,42,42	0
55	MG	1A	3747	1/1	0.94	0.20	27,27,27,27	0
55	MG	1A	3748	1/1	0.94	0.13	49,49,49,49	0
55	MG	1a	1815	1/1	0.94	0.09	93,93,93,93	0
55	MG	1a	1818	1/1	0.94	0.14	72,72,72,72	0
55	MG	1A	3955	1/1	0.94	0.19	19,19,19,19	0
56	ZN	2n	101	1/1	0.94	0.07	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1A	3559	1/1	0.95	0.52	15,15,15,15	0
55	MG	1A	3124	1/1	0.95	0.44	28,28,28,28	0
55	MG	1A	3215	1/1	0.95	0.35	23,23,23,23	0
55	MG	2T	201	1/1	0.95	0.14	21,21,21,21	0
55	MG	2T	203	1/1	0.95	0.76	59,59,59,59	0
55	MG	1a	1654	1/1	0.95	0.39	46,46,46,46	0
55	MG	1A	3792	1/1	0.95	0.18	25,25,25,25	0
55	MG	1B	222	1/1	0.95	0.10	35,35,35,35	0
55	MG	1A	3217	1/1	0.95	0.16	62,62,62,62	0
55	MG	1A	3479	1/1	0.95	0.09	39,39,39,39	0
55	MG	1A	3218	1/1	0.95	0.24	46,46,46,46	0
55	MG	2V	205	1/1	0.95	0.13	59,59,59,59	0
55	MG	1A	3016	1/1	0.95	0.73	15,15,15,15	0
55	MG	1A	3801	1/1	0.95	0.07	83,83,83,83	0
55	MG	1A	3567	1/1	0.95	0.17	12,12,12,12	0
55	MG	1a	1664	1/1	0.95	0.31	67,67,67,67	0
55	MG	1A	3675	1/1	0.95	0.25	44,44,44,44	0
55	MG	1A	3049	1/1	0.95	0.26	22,22,22,22	0
55	MG	1A	3050	1/1	0.95	0.47	29,29,29,29	0
55	MG	2A	3767	1/1	0.95	0.10	52,52,52,52	0
55	MG	1A	3006	1/1	0.95	0.16	21,21,21,21	0
55	MG	1A	3279	1/1	0.95	0.16	70,70,70,70	0
55	MG	2A	3770	1/1	0.95	0.20	47,47,47,47	0
55	MG	1A	3681	1/1	0.95	0.13	38,38,38,38	0
55	MG	1A	3825	1/1	0.95	0.05	18,18,18,18	0
55	MG	25	104	1/1	0.95	0.95	33,33,33,33	0
55	MG	1A	3052	1/1	0.95	0.61	34,34,34,34	0
55	MG	1A	3828	1/1	0.95	0.12	52,52,52,52	0
55	MG	2A	3778	1/1	0.95	0.07	63,63,63,63	0
55	MG	29	102	1/1	0.95	1.40	48,48,48,48	0
55	MG	2A	3516	1/1	0.95	0.05	65,65,65,65	0
55	MG	2A	3517	1/1	0.95	0.16	48,48,48,48	0
55	MG	2A	3518	1/1	0.95	0.14	58,58,58,58	0
55	MG	2a	1604	1/1	0.95	0.14	81,81,81,81	0
55	MG	1A	3830	1/1	0.95	0.81	21,21,21,21	0
55	MG	2A	3520	1/1	0.95	0.13	54,54,54,54	0
55	MG	2A	3785	1/1	0.95	0.16	71,71,71,71	0
55	MG	2A	3786	1/1	0.95	0.31	50,50,50,50	0
55	MG	2A	3220	1/1	0.95	0.20	58,58,58,58	0
55	MG	1A	3832	1/1	0.95	0.22	10,10,10,10	0
55	MG	1A	3131	1/1	0.95	0.30	19,19,19,19	0
55	MG	1a	1678	1/1	0.95	0.05	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1E	304	1/1	0.95	0.13	25,25,25,25	0
55	MG	2A	3798	1/1	0.95	0.18	60,60,60,60	0
55	MG	1A	3838	1/1	0.95	0.22	39,39,39,39	0
55	MG	1A	3287	1/1	0.95	0.07	26,26,26,26	0
55	MG	2A	3801	1/1	0.95	0.13	57,57,57,57	0
55	MG	2A	3802	1/1	0.95	0.07	45,45,45,45	0
55	MG	2A	3005	1/1	0.95	0.24	37,37,37,37	0
55	MG	2a	1622	1/1	0.95	0.27	51,51,51,51	0
55	MG	1A	3391	1/1	0.95	0.24	30,30,30,30	0
55	MG	1a	1683	1/1	0.95	0.22	72,72,72,72	0
55	MG	2A	3809	1/1	0.95	0.08	35,35,35,35	0
55	MG	1A	3844	1/1	0.95	0.06	53,53,53,53	0
55	MG	2A	3242	1/1	0.95	0.22	32,32,32,32	0
55	MG	1F	305	1/1	0.95	0.67	18,18,18,18	0
55	MG	1A	3845	1/1	0.95	0.15	47,47,47,47	0
55	MG	1A	3019	1/1	0.95	0.40	15,15,15,15	0
55	MG	1A	3396	1/1	0.95	0.23	35,35,35,35	0
55	MG	2A	3540	1/1	0.95	0.13	49,49,49,49	0
55	MG	2a	1633	1/1	0.95	0.13	47,47,47,47	0
55	MG	1A	3696	1/1	0.95	0.13	50,50,50,50	0
55	MG	1F	312	1/1	0.95	0.73	22,22,22,22	0
55	MG	1A	3697	1/1	0.95	0.32	37,37,37,37	0
55	MG	1A	3499	1/1	0.95	0.07	33,33,33,33	0
55	MG	2a	1638	1/1	0.95	0.29	50,50,50,50	0
55	MG	2A	3546	1/1	0.95	0.13	52,52,52,52	0
55	MG	1a	1701	1/1	0.95	0.07	56,56,56,56	0
55	MG	1A	3590	1/1	0.95	0.10	47,47,47,47	0
55	MG	1A	3084	1/1	0.95	0.08	48,48,48,48	0
55	MG	2A	3552	1/1	0.95	0.75	40,40,40,40	0
55	MG	1A	3185	1/1	0.95	0.37	25,25,25,25	0
55	MG	1H	201	1/1	0.95	0.20	47,47,47,47	0
55	MG	1A	3861	1/1	0.95	0.20	63,63,63,63	0
55	MG	2a	1648	1/1	0.95	0.23	42,42,42,42	0
55	MG	2a	1649	1/1	0.95	0.13	65,65,65,65	0
55	MG	1N	203	1/1	0.95	0.48	55,55,55,55	0
55	MG	1N	204	1/1	0.95	0.25	73,73,73,73	0
55	MG	1A	3187	1/1	0.95	0.30	28,28,28,28	0
55	MG	2A	3263	1/1	0.95	0.12	44,44,44,44	0
55	MG	2a	1656	1/1	0.95	0.18	76,76,76,76	0
55	MG	1A	3155	1/1	0.95	0.29	16,16,16,16	0
55	MG	1A	3189	1/1	0.95	0.94	30,30,30,30	0
55	MG	2A	3848	1/1	0.95	0.16	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3711	1/1	0.95	0.08	21,21,21,21	0
55	MG	1a	1718	1/1	0.95	0.08	48,48,48,48	0
55	MG	1A	3414	1/1	0.95	0.09	29,29,29,29	0
55	MG	1A	3311	1/1	0.95	0.20	11,11,11,11	0
55	MG	2A	3041	1/1	0.95	0.11	46,46,46,46	0
55	MG	1a	1722	1/1	0.95	0.08	63,63,63,63	0
55	MG	2A	3043	1/1	0.95	0.52	35,35,35,35	0
55	MG	1A	3869	1/1	0.95	0.30	38,38,38,38	0
55	MG	2A	3283	1/1	0.95	0.16	61,61,61,61	0
55	MG	2A	3863	1/1	0.95	0.12	61,61,61,61	0
55	MG	1A	3417	1/1	0.95	0.11	32,32,32,32	0
55	MG	1a	1727	1/1	0.95	0.13	77,77,77,77	0
55	MG	2A	3289	1/1	0.95	0.14	64,64,64,64	0
55	MG	2A	3291	1/1	0.95	0.10	29,29,29,29	0
55	MG	2A	3293	1/1	0.95	0.23	7,7,7,7	0
55	MG	1A	3001	1/1	0.95	0.11	23,23,23,23	0
55	MG	1A	3422	1/1	0.95	0.15	42,42,42,42	0
55	MG	2A	3296	1/1	0.95	0.23	54,54,54,54	0
55	MG	1A	3608	1/1	0.95	0.06	49,49,49,49	0
55	MG	1a	1733	1/1	0.95	0.35	67,67,67,67	0
55	MG	1A	3086	1/1	0.95	0.48	38,38,38,38	0
55	MG	2A	3056	1/1	0.95	0.09	54,54,54,54	0
55	MG	1A	3192	1/1	0.95	0.52	31,31,31,31	0
55	MG	2A	3877	1/1	0.95	0.10	26,26,26,26	0
55	MG	2A	3878	1/1	0.95	0.51	43,43,43,43	0
55	MG	2A	3879	1/1	0.95	0.11	38,38,38,38	0
55	MG	2A	3058	1/1	0.95	0.09	59,59,59,59	0
55	MG	1a	1738	1/1	0.95	0.21	50,50,50,50	0
55	MG	1A	3247	1/1	0.95	0.25	41,41,41,41	0
55	MG	2a	1696	1/1	0.95	0.10	38,38,38,38	0
55	MG	2A	3597	1/1	0.95	0.16	52,52,52,52	0
55	MG	2a	1698	1/1	0.95	0.06	75,75,75,75	0
55	MG	2A	3598	1/1	0.95	0.49	34,34,34,34	0
55	MG	1A	3880	1/1	0.95	0.23	54,54,54,54	0
55	MG	2A	3886	1/1	0.95	0.17	55,55,55,55	0
55	MG	2A	3601	1/1	0.95	0.13	34,34,34,34	0
55	MG	1A	3160	1/1	0.95	0.90	23,23,23,23	0
55	MG	2a	1704	1/1	0.95	0.21	63,63,63,63	0
55	MG	2A	3604	1/1	0.95	0.15	49,49,49,49	0
55	MG	1A	3439	1/1	0.95	0.05	49,49,49,49	0
55	MG	2a	1708	1/1	0.95	0.13	76,76,76,76	0
55	MG	1A	3440	1/1	0.95	0.09	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3607	1/1	0.95	0.09	74,74,74,74	0
55	MG	2A	3895	1/1	0.95	0.17	55,55,55,55	0
55	MG	2a	1716	1/1	0.95	0.08	55,55,55,55	0
55	MG	2A	3321	1/1	0.95	0.20	30,30,30,30	0
55	MG	2A	3609	1/1	0.95	0.20	64,64,64,64	0
55	MG	10	106	1/1	0.95	0.20	39,39,39,39	0
55	MG	2A	3902	1/1	0.95	0.22	87,87,87,87	0
55	MG	1A	3884	1/1	0.95	0.14	76,76,76,76	0
55	MG	1A	3886	1/1	0.95	0.08	38,38,38,38	0
55	MG	1a	1747	1/1	0.95	0.20	36,36,36,36	0
55	MG	2A	3328	1/1	0.95	0.24	39,39,39,39	0
55	MG	11	103	1/1	0.95	0.14	44,44,44,44	0
55	MG	1A	3523	1/1	0.95	0.13	12,12,12,12	0
55	MG	1A	3619	1/1	0.95	0.17	45,45,45,45	0
55	MG	2A	3080	1/1	0.95	0.23	55,55,55,55	0
55	MG	2a	1731	1/1	0.95	0.10	62,62,62,62	0
55	MG	2A	3622	1/1	0.95	0.15	46,46,46,46	0
55	MG	1A	3620	1/1	0.95	0.12	58,58,58,58	0
55	MG	2A	3082	1/1	0.95	0.17	50,50,50,50	0
55	MG	1A	3527	1/1	0.95	0.16	40,40,40,40	0
55	MG	2a	1737	1/1	0.95	0.17	73,73,73,73	0
55	MG	2A	3337	1/1	0.95	0.14	22,22,22,22	0
55	MG	2A	3627	1/1	0.95	0.20	68,68,68,68	0
55	MG	2A	3339	1/1	0.95	0.09	34,34,34,34	0
55	MG	2A	3341	1/1	0.95	0.40	32,32,32,32	0
55	MG	2a	1743	1/1	0.95	0.13	75,75,75,75	0
55	MG	1A	3442	1/1	0.95	0.14	25,25,25,25	0
55	MG	1A	3089	1/1	0.95	0.54	26,26,26,26	0
55	MG	2A	3633	1/1	0.95	0.14	17,17,17,17	0
55	MG	1A	3735	1/1	0.95	0.20	63,63,63,63	0
55	MG	1A	3736	1/1	0.95	0.18	33,33,33,33	0
55	MG	1A	3738	1/1	0.95	0.12	19,19,19,19	0
55	MG	2a	1750	1/1	0.95	0.12	72,72,72,72	0
55	MG	2A	3096	1/1	0.95	0.16	35,35,35,35	0
55	MG	1A	3624	1/1	0.95	0.20	58,58,58,58	0
55	MG	1A	3625	1/1	0.95	0.11	69,69,69,69	0
55	MG	2A	3361	1/1	0.95	0.10	26,26,26,26	0
55	MG	1A	3323	1/1	0.95	0.14	24,24,24,24	0
55	MG	2A	3368	1/1	0.95	0.24	51,51,51,51	0
55	MG	1a	1761	1/1	0.95	0.17	72,72,72,72	0
55	MG	2A	3940	1/1	0.95	0.10	48,48,48,48	0
55	MG	1a	1762	1/1	0.95	0.13	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	2A	3373	1/1	0.95	0.10	27,27,27,27	0
55	MG	1A	3627	1/1	0.95	0.11	62,62,62,62	0
55	MG	2A	3104	1/1	0.95	0.17	57,57,57,57	0
55	MG	1A	3535	1/1	0.95	0.14	19,19,19,19	0
55	MG	1A	3632	1/1	0.95	0.26	16,16,16,16	0
55	MG	1a	1604	1/1	0.95	0.18	73,73,73,73	0
55	MG	1a	1605	1/1	0.95	0.12	60,60,60,60	0
55	MG	2A	3952	1/1	0.95	0.13	27,27,27,27	0
55	MG	1a	1606	1/1	0.95	0.15	53,53,53,53	0
55	MG	2A	3386	1/1	0.95	0.08	44,44,44,44	0
55	MG	1A	3022	1/1	0.95	0.34	42,42,42,42	0
55	MG	1A	3915	1/1	0.95	0.19	63,63,63,63	0
55	MG	1A	3057	1/1	0.95	0.26	16,16,16,16	0
55	MG	1A	3013	1/1	0.95	0.17	17,17,17,17	0
55	MG	2a	1777	1/1	0.95	0.28	55,55,55,55	0
55	MG	2A	3960	1/1	0.95	0.36	44,44,44,44	0
55	MG	1A	3753	1/1	0.95	0.35	49,49,49,49	0
55	MG	1A	3165	1/1	0.95	0.69	25,25,25,25	0
55	MG	1A	3755	1/1	0.95	0.10	58,58,58,58	0
55	MG	1A	3927	1/1	0.95	0.14	27,27,27,27	0
55	MG	1A	3541	1/1	0.95	0.08	41,41,41,41	0
55	MG	1a	1617	1/1	0.95	0.19	93,93,93,93	0
55	MG	1a	1781	1/1	0.95	0.21	63,63,63,63	0
55	MG	1A	3758	1/1	0.95	0.20	17,17,17,17	0
55	MG	1A	3759	1/1	0.95	0.08	28,28,28,28	0
55	MG	1A	3939	1/1	0.95	0.21	24,24,24,24	0
55	MG	2A	3678	1/1	0.95	0.23	53,53,53,53	0
55	MG	1A	3333	1/1	0.95	0.14	28,28,28,28	0
55	MG	2A	3412	1/1	0.95	0.37	68,68,68,68	0
55	MG	2a	1792	1/1	0.95	0.14	56,56,56,56	0
55	MG	1a	1622	1/1	0.95	0.25	59,59,59,59	0
55	MG	2A	3138	1/1	0.95	0.28	40,40,40,40	0
55	MG	1A	3943	1/1	0.95	0.93	34,34,34,34	0
55	MG	2A	3418	1/1	0.95	0.04	60,60,60,60	0
55	MG	2a	1797	1/1	0.95	0.10	75,75,75,75	0
55	MG	1A	3643	1/1	0.95	0.21	40,40,40,40	0
55	MG	2A	3143	1/1	0.95	0.52	42,42,42,42	0
55	MG	1A	3203	1/1	0.95	0.17	34,34,34,34	0
55	MG	1A	3546	1/1	0.95	0.11	48,48,48,48	0
55	MG	2A	3147	1/1	0.95	0.42	38,38,38,38	0
55	MG	2A	3148	1/1	0.95	0.48	35,35,35,35	0
55	MG	1A	3949	1/1	0.95	0.56	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	2A	3438	1/1	0.95	0.16	38,38,38,38	0
55	MG	1A	3547	1/1	0.95	0.11	29,29,29,29	0
55	MG	2B	3020	1/1	0.95	0.07	58,58,58,58	0
55	MG	1A	3339	1/1	0.95	0.14	13,13,13,13	0
55	MG	1a	1631	1/1	0.95	0.08	61,61,61,61	0
55	MG	2A	3442	1/1	0.95	0.15	20,20,20,20	0
55	MG	1A	3953	1/1	0.95	0.63	22,22,22,22	0
55	MG	2A	3154	1/1	0.95	0.22	44,44,44,44	0
55	MG	2a	1815	1/1	0.95	0.09	75,75,75,75	0
55	MG	1a	1633	1/1	0.95	0.12	34,34,34,34	0
55	MG	2a	1822	1/1	0.95	0.39	51,51,51,51	0
55	MG	2D	305	1/1	0.95	0.46	33,33,33,33	0
55	MG	2a	1826	1/1	0.95	0.25	85,85,85,85	0
55	MG	1A	3954	1/1	0.95	0.33	21,21,21,21	0
55	MG	2A	3707	1/1	0.95	0.11	26,26,26,26	0
55	MG	2A	3450	1/1	0.95	0.56	28,28,28,28	0
55	MG	2A	3451	1/1	0.95	0.17	30,30,30,30	0
55	MG	1A	3549	1/1	0.95	0.19	40,40,40,40	0
55	MG	2a	1833	1/1	0.95	0.07	71,71,71,71	0
55	MG	1A	3259	1/1	0.95	0.14	17,17,17,17	0
55	MG	1a	1637	1/1	0.95	1.17	57,57,57,57	0
55	MG	1A	3776	1/1	0.95	0.08	46,46,46,46	0
55	MG	1A	3343	1/1	0.95	0.06	12,12,12,12	0
55	MG	1A	3093	1/1	0.95	0.24	27,27,27,27	0
55	MG	2A	3460	1/1	0.95	0.14	25,25,25,25	0
55	MG	1a	1811	1/1	0.95	0.11	61,61,61,61	0
55	MG	1A	3347	1/1	0.95	0.18	13,13,13,13	0
55	MG	2A	3725	1/1	0.95	0.15	40,40,40,40	0
55	MG	1a	1814	1/1	0.95	0.10	54,54,54,54	0
55	MG	2A	3468	1/1	0.95	0.11	36,36,36,36	0
55	MG	2F	303	1/1	0.95	0.88	40,40,40,40	0
55	MG	2f	8001	1/1	0.95	0.12	75,75,75,75	0
55	MG	2A	3728	1/1	0.95	0.12	37,37,37,37	0
55	MG	1B	206	1/1	0.95	0.14	50,50,50,50	0
55	MG	2A	3470	1/1	0.95	0.14	26,26,26,26	0
55	MG	1a	1645	1/1	0.95	0.29	64,64,64,64	0
55	MG	1a	1819	1/1	0.95	0.06	52,52,52,52	0
55	MG	1B	207	1/1	0.95	0.39	41,41,41,41	0
55	MG	1a	1825	1/1	0.95	0.13	71,71,71,71	0
55	MG	1A	3211	1/1	0.95	0.47	20,20,20,20	0
55	MG	2A	3736	1/1	0.95	0.08	52,52,52,52	0
55	MG	2A	3481	1/1	0.95	0.86	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1A	3470	1/1	0.95	0.17	20,20,20,20	0
55	MG	1a	1829	1/1	0.95	0.07	84,84,84,84	0
55	MG	1A	3003	1/1	0.95	0.11	21,21,21,21	0
55	MG	2A	3485	1/1	0.95	0.17	60,60,60,60	0
55	MG	1B	212	1/1	0.95	0.05	59,59,59,59	0
55	MG	1a	1842	1/1	0.96	0.11	56,56,56,56	0
55	MG	1T	202	1/1	0.96	0.50	60,60,60,60	0
55	MG	2A	3166	1/1	0.96	0.40	36,36,36,36	0
55	MG	1A	3324	1/1	0.96	0.06	52,52,52,52	0
55	MG	1A	3897	1/1	0.96	0.12	45,45,45,45	0
55	MG	2A	3398	1/1	0.96	0.18	47,47,47,47	0
55	MG	1A	3571	1/1	0.96	0.09	55,55,55,55	0
55	MG	1A	3011	1/1	0.96	0.13	27,27,27,27	0
55	MG	1A	3327	1/1	0.96	0.14	23,23,23,23	0
55	MG	1a	1693	1/1	0.96	0.24	44,44,44,44	0
55	MG	1A	3667	1/1	0.96	0.09	41,41,41,41	0
55	MG	2A	3409	1/1	0.96	0.17	46,46,46,46	0
55	MG	1a	1695	1/1	0.96	0.14	53,53,53,53	0
55	MG	2A	3411	1/1	0.96	0.20	49,49,49,49	0
55	MG	2A	3632	1/1	0.96	0.07	74,74,74,74	0
55	MG	1a	1696	1/1	0.96	0.29	63,63,63,63	0
55	MG	1A	3577	1/1	0.96	0.16	20,20,20,20	0
55	MG	1A	3764	1/1	0.96	0.05	45,45,45,45	0
55	MG	1A	3202	1/1	0.96	0.63	29,29,29,29	0
55	MG	1A	3907	1/1	0.96	0.80	20,20,20,20	0
55	MG	2A	3183	1/1	0.96	0.16	43,43,43,43	0
55	MG	2A	3420	1/1	0.96	0.09	50,50,50,50	0
55	MG	1A	3908	1/1	0.96	0.34	14,14,14,14	0
55	MG	2A	3185	1/1	0.96	0.47	51,51,51,51	0
55	MG	1A	3767	1/1	0.96	0.06	42,42,42,42	0
55	MG	2A	3428	1/1	0.96	0.35	62,62,62,62	0
55	MG	10	101	1/1	0.96	0.13	36,36,36,36	0
55	MG	2A	3647	1/1	0.96	0.87	37,37,37,37	0
55	MG	1A	3768	1/1	0.96	0.12	25,25,25,25	0
55	MG	2A	3436	1/1	0.96	0.07	47,47,47,47	0
55	MG	1A	3670	1/1	0.96	0.45	36,36,36,36	0
55	MG	1A	3183	1/1	0.96	0.51	39,39,39,39	0
55	MG	1A	3502	1/1	0.96	0.30	36,36,36,36	0
55	MG	2A	3653	1/1	0.96	0.37	76,76,76,76	0
55	MG	2A	3654	1/1	0.96	0.28	37,37,37,37	0
55	MG	2A	3896	1/1	0.96	0.29	45,45,45,45	0
55	MG	1A	3775	1/1	0.96	0.14	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	11	101	1/1	0.96	0.14	26,26,26,26	0
55	MG	1A	3418	1/1	0.96	0.09	53,53,53,53	0
55	MG	2A	3443	1/1	0.96	0.07	25,25,25,25	0
55	MG	1a	1719	1/1	0.96	0.05	44,44,44,44	0
55	MG	1A	3238	1/1	0.96	0.24	20,20,20,20	0
55	MG	2A	3662	1/1	0.96	0.18	46,46,46,46	0
55	MG	2a	1667	1/1	0.96	0.39	52,52,52,52	0
55	MG	1A	3420	1/1	0.96	0.09	48,48,48,48	0
55	MG	13	101	1/1	0.96	0.19	30,30,30,30	0
55	MG	1A	3779	1/1	0.96	0.15	17,17,17,17	0
55	MG	1A	3922	1/1	0.96	0.12	31,31,31,31	0
55	MG	1a	1725	1/1	0.96	0.23	47,47,47,47	0
55	MG	1A	3332	1/1	0.96	0.16	53,53,53,53	0
55	MG	2a	1674	1/1	0.96	0.22	31,31,31,31	0
55	MG	1a	1728	1/1	0.96	0.08	69,69,69,69	0
55	MG	1a	1729	1/1	0.96	0.47	43,43,43,43	0
55	MG	2A	3211	1/1	0.96	0.42	40,40,40,40	0
55	MG	2A	3023	1/1	0.96	0.69	44,44,44,44	0
55	MG	1A	3925	1/1	0.96	0.35	26,26,26,26	0
55	MG	15	105	1/1	0.96	0.56	36,36,36,36	0
55	MG	2A	3217	1/1	0.96	0.48	32,32,32,32	0
55	MG	1A	3507	1/1	0.96	0.18	47,47,47,47	0
55	MG	1A	3204	1/1	0.96	0.18	31,31,31,31	0
55	MG	17	102	1/1	0.96	0.16	28,28,28,28	0
55	MG	2A	3928	1/1	0.96	0.10	35,35,35,35	0
55	MG	1A	3931	1/1	0.96	0.10	32,32,32,32	0
55	MG	2a	1687	1/1	0.96	0.18	67,67,67,67	0
55	MG	1a	1737	1/1	0.96	0.10	67,67,67,67	0
55	MG	1A	3932	1/1	0.96	0.64	24,24,24,24	0
55	MG	1A	3510	1/1	0.96	0.04	57,57,57,57	0
55	MG	2a	1691	1/1	0.96	0.30	59,59,59,59	0
55	MG	2a	1692	1/1	0.96	0.14	61,61,61,61	0
55	MG	2a	1693	1/1	0.96	0.29	67,67,67,67	0
55	MG	1A	3935	1/1	0.96	0.72	20,20,20,20	0
55	MG	2a	1695	1/1	0.96	0.06	48,48,48,48	0
55	MG	2A	3688	1/1	0.96	0.18	51,51,51,51	0
55	MG	2A	3476	1/1	0.96	0.14	56,56,56,56	0
55	MG	19	102	1/1	0.96	0.24	50,50,50,50	0
55	MG	1A	3937	1/1	0.96	0.41	19,19,19,19	0
55	MG	1A	3683	1/1	0.96	0.06	73,73,73,73	0
55	MG	2A	3236	1/1	0.96	0.07	91,91,91,91	0
55	MG	2A	3695	1/1	0.96	0.21	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3428	1/1	0.96	0.10	12,12,12,12	0
55	MG	2A	3697	1/1	0.96	0.28	33,33,33,33	0
55	MG	1A	3787	1/1	0.96	0.10	23,23,23,23	0
55	MG	1A	3431	1/1	0.96	0.10	14,14,14,14	0
55	MG	2a	1707	1/1	0.96	0.07	51,51,51,51	0
55	MG	1A	3944	1/1	0.96	0.75	28,28,28,28	0
55	MG	1A	3014	1/1	0.96	0.18	28,28,28,28	0
55	MG	1A	3690	1/1	0.96	0.54	33,33,33,33	0
55	MG	1A	3336	1/1	0.96	0.12	37,37,37,37	0
55	MG	1A	3948	1/1	0.96	0.56	24,24,24,24	0
55	MG	1A	3272	1/1	0.96	0.77	22,22,22,22	0
55	MG	1A	3438	1/1	0.96	0.06	33,33,33,33	0
55	MG	1A	3604	1/1	0.96	0.09	25,25,25,25	0
55	MG	2A	3054	1/1	0.96	0.17	31,31,31,31	0
55	MG	1A	3802	1/1	0.96	0.12	26,26,26,26	0
55	MG	1A	3241	1/1	0.96	0.82	21,21,21,21	0
55	MG	1A	3606	1/1	0.96	0.10	23,23,23,23	0
55	MG	1A	3811	1/1	0.96	0.07	13,13,13,13	0
55	MG	2A	3505	1/1	0.96	0.16	47,47,47,47	0
55	MG	1A	3029	1/1	0.96	0.10	21,21,21,21	0
55	MG	1A	3813	1/1	0.96	0.15	26,26,26,26	0
55	MG	1A	3276	1/1	0.96	0.10	35,35,35,35	0
55	MG	2A	3722	1/1	0.96	0.18	63,63,63,63	0
55	MG	1A	3701	1/1	0.96	0.07	33,33,33,33	0
55	MG	2a	1733	1/1	0.96	0.42	47,47,47,47	0
55	MG	2A	3724	1/1	0.96	0.05	63,63,63,63	0
55	MG	1A	3816	1/1	0.96	0.22	43,43,43,43	0
55	MG	1A	3186	1/1	0.96	0.65	24,24,24,24	0
55	MG	1A	3703	1/1	0.96	0.08	17,17,17,17	0
55	MG	1A	3704	1/1	0.96	0.07	57,57,57,57	0
55	MG	2A	3514	1/1	0.96	0.16	59,59,59,59	0
55	MG	1B	210	1/1	0.96	0.51	52,52,52,52	0
55	MG	1A	3056	1/1	0.96	0.13	50,50,50,50	0
55	MG	2a	1742	1/1	0.96	0.17	51,51,51,51	0
55	MG	1A	3708	1/1	0.96	0.05	32,32,32,32	0
55	MG	2A	3276	1/1	0.96	0.47	41,41,41,41	0
55	MG	1A	3357	1/1	0.96	0.31	40,40,40,40	0
55	MG	1A	3284	1/1	0.96	0.32	34,34,34,34	0
55	MG	1A	3833	1/1	0.96	0.15	17,17,17,17	0
55	MG	2A	3737	1/1	0.96	0.08	43,43,43,43	0
55	MG	1A	3448	1/1	0.96	0.17	41,41,41,41	0
55	MG	1B	221	1/1	0.96	0.07	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	2A	3285	1/1	0.96	0.10	27,27,27,27	0
55	MG	1A	3359	1/1	0.96	0.12	46,46,46,46	0
55	MG	2A	3288	1/1	0.96	0.12	24,24,24,24	0
55	MG	1A	3714	1/1	0.96	0.15	26,26,26,26	0
55	MG	1A	3360	1/1	0.96	0.12	16,16,16,16	0
55	MG	2A	3089	1/1	0.96	0.39	49,49,49,49	0
55	MG	1a	1638	1/1	0.96	0.20	30,30,30,30	0
55	MG	2a	1758	1/1	0.96	0.12	75,75,75,75	0
55	MG	1A	3618	1/1	0.96	0.50	24,24,24,24	0
55	MG	1A	3454	1/1	0.96	0.14	9,9,9,9	0
55	MG	2A	3094	1/1	0.96	0.94	42,42,42,42	0
55	MG	2D	306	1/1	0.96	0.44	33,33,33,33	0
55	MG	2A	3536	1/1	0.96	0.30	58,58,58,58	0
55	MG	2A	3095	1/1	0.96	0.18	17,17,17,17	0
55	MG	1A	3361	1/1	0.96	0.12	35,35,35,35	0
55	MG	2D	310	1/1	0.96	0.27	40,40,40,40	0
55	MG	2a	1768	1/1	0.96	0.22	59,59,59,59	0
55	MG	1A	3245	1/1	0.96	0.09	65,65,65,65	0
55	MG	1A	3246	1/1	0.96	0.32	32,32,32,32	0
55	MG	2A	3306	1/1	0.96	0.14	46,46,46,46	0
55	MG	2A	3762	1/1	0.96	0.15	69,69,69,69	0
55	MG	1A	3849	1/1	0.96	0.08	39,39,39,39	0
55	MG	1A	3098	1/1	0.96	0.50	34,34,34,34	0
55	MG	1A	3854	1/1	0.96	0.25	38,38,38,38	0
55	MG	2A	3545	1/1	0.96	0.19	39,39,39,39	0
55	MG	1A	3248	1/1	0.96	0.33	39,39,39,39	0
55	MG	1a	1793	1/1	0.96	0.16	77,77,77,77	0
55	MG	1D	310	1/1	0.96	0.28	10,10,10,10	0
55	MG	1A	3462	1/1	0.96	0.25	50,50,50,50	0
55	MG	1A	3291	1/1	0.96	0.19	45,45,45,45	0
55	MG	2F	302	1/1	0.96	0.38	35,35,35,35	0
55	MG	1A	3216	1/1	0.96	0.34	21,21,21,21	0
55	MG	2A	3111	1/1	0.96	0.50	44,44,44,44	0
55	MG	2F	306	1/1	0.96	0.48	34,34,34,34	0
55	MG	1A	3251	1/1	0.96	0.69	16,16,16,16	0
55	MG	1A	3171	1/1	0.96	0.29	24,24,24,24	0
55	MG	1A	3067	1/1	0.96	0.27	27,27,27,27	0
55	MG	2A	3115	1/1	0.96	0.30	31,31,31,31	0
55	MG	1A	3308	1/1	0.96	0.13	17,17,17,17	0
55	MG	1A	3117	1/1	0.96	0.04	72,72,72,72	0
55	MG	1A	3637	1/1	0.96	0.12	36,36,36,36	0
55	MG	1A	3101	1/1	0.96	0.40	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	2N	201	1/1	0.96	0.20	72,72,72,72	0
55	MG	1A	3555	1/1	0.96	0.14	27,27,27,27	0
55	MG	1F	303	1/1	0.96	0.45	56,56,56,56	0
55	MG	1A	3737	1/1	0.96	0.07	53,53,53,53	0
55	MG	2A	3790	1/1	0.96	0.09	52,52,52,52	0
55	MG	1A	3478	1/1	0.96	0.11	36,36,36,36	0
55	MG	2A	3340	1/1	0.96	0.12	39,39,39,39	0
55	MG	1a	1665	1/1	0.96	0.49	75,75,75,75	0
55	MG	2A	3796	1/1	0.96	0.19	79,79,79,79	0
55	MG	2A	3129	1/1	0.96	0.99	33,33,33,33	0
55	MG	1A	3008	1/1	0.96	0.15	32,32,32,32	0
55	MG	2T	202	1/1	0.96	0.07	56,56,56,56	0
55	MG	1A	3875	1/1	0.96	0.44	26,26,26,26	0
55	MG	2a	1807	1/1	0.96	0.08	55,55,55,55	0
55	MG	2A	3346	1/1	0.96	0.09	35,35,35,35	0
55	MG	2A	3573	1/1	0.96	0.21	27,27,27,27	0
55	MG	2A	3574	1/1	0.96	0.07	47,47,47,47	0
55	MG	2a	1811	1/1	0.96	0.06	60,60,60,60	0
55	MG	1a	1817	1/1	0.96	0.11	65,65,65,65	0
55	MG	2A	3805	1/1	0.96	0.09	73,73,73,73	0
55	MG	2A	3577	1/1	0.96	0.06	69,69,69,69	0
55	MG	2A	3579	1/1	0.96	0.13	37,37,37,37	0
55	MG	2a	1817	1/1	0.96	0.21	68,68,68,68	0
55	MG	2a	1819	1/1	0.96	0.14	61,61,61,61	0
55	MG	1A	3226	1/1	0.96	0.23	27,27,27,27	0
55	MG	1A	3395	1/1	0.96	0.38	34,34,34,34	0
55	MG	2A	3583	1/1	0.96	0.07	50,50,50,50	0
55	MG	2A	3584	1/1	0.96	0.88	33,33,33,33	0
55	MG	2A	3816	1/1	0.96	0.10	42,42,42,42	0
55	MG	2A	3353	1/1	0.96	0.14	24,24,24,24	0
55	MG	1A	3044	1/1	0.96	0.16	21,21,21,21	0
55	MG	2A	3358	1/1	0.96	0.10	23,23,23,23	0
55	MG	2A	3139	1/1	0.96	0.32	38,38,38,38	0
55	MG	1a	1822	1/1	0.96	0.40	74,74,74,74	0
55	MG	2A	3362	1/1	0.96	0.11	32,32,32,32	0
55	MG	2A	3363	1/1	0.96	0.22	50,50,50,50	0
55	MG	1a	1824	1/1	0.96	0.13	42,42,42,42	0
55	MG	2A	3366	1/1	0.96	0.12	25,25,25,25	0
55	MG	1A	3025	1/1	0.96	1.08	22,22,22,22	0
55	MG	1A	3485	1/1	0.96	0.72	30,30,30,30	0
55	MG	1A	3178	1/1	0.96	0.12	34,34,34,34	0
55	MG	1A	3653	1/1	0.96	0.64	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	1830	1/1	0.96	0.20	56,56,56,56	0
55	MG	2a	1601	1/1	0.96	0.10	66,66,66,66	0
55	MG	1A	3403	1/1	0.96	0.09	40,40,40,40	0
55	MG	1A	3565	1/1	0.96	0.14	42,42,42,42	0
55	MG	2A	3838	1/1	0.96	0.09	48,48,48,48	0
55	MG	1A	3885	1/1	0.96	0.10	47,47,47,47	0
55	MG	1N	202	1/1	0.96	0.51	32,32,32,32	0
55	MG	1A	3179	1/1	0.96	0.15	51,51,51,51	0
55	MG	2a	1609	1/1	0.96	0.21	78,78,78,78	0
55	MG	2A	3383	1/1	0.96	0.07	46,46,46,46	0
55	MG	2A	3846	1/1	0.96	0.09	56,56,56,56	0
55	MG	1A	3887	1/1	0.96	0.25	71,71,71,71	0
55	MG	2A	3385	1/1	0.96	0.12	40,40,40,40	0
55	MG	1A	3406	1/1	0.96	0.09	38,38,38,38	0
55	MG	1A	3408	1/1	0.96	0.08	54,54,54,54	0
55	MG	2A	3852	1/1	0.96	0.28	50,50,50,50	0
55	MG	1a	1839	1/1	0.96	0.13	56,56,56,56	0
55	MG	2A	3855	1/1	0.96	0.04	64,64,64,64	0
56	ZN	1n	501	1/1	0.96	0.12	75,75,75,75	0
56	ZN	2Y	202	1/1	0.96	0.05	80,80,80,80	0
55	MG	1A	3757	1/1	0.96	0.16	9,9,9,9	0
55	MG	1R	204	1/1	0.96	0.21	19,19,19,19	0
55	MG	1A	3412	1/1	0.97	0.04	50,50,50,50	0
55	MG	2A	3063	1/1	0.97	0.14	32,32,32,32	0
55	MG	1A	3043	1/1	0.97	0.41	10,10,10,10	0
55	MG	2A	3771	1/1	0.97	0.15	46,46,46,46	0
55	MG	1A	3277	1/1	0.97	0.16	37,37,37,37	0
55	MG	1B	202	1/1	0.97	0.24	52,52,52,52	0
55	MG	2A	3067	1/1	0.97	0.25	41,41,41,41	0
55	MG	1a	1764	1/1	0.97	0.11	75,75,75,75	0
55	MG	2A	3275	1/1	0.97	0.23	47,47,47,47	0
55	MG	1A	3060	1/1	0.97	0.16	22,22,22,22	0
55	MG	2A	3780	1/1	0.97	0.13	29,29,29,29	0
55	MG	1A	3595	1/1	0.97	0.12	27,27,27,27	0
55	MG	25	101	1/1	0.97	0.11	48,48,48,48	0
55	MG	1A	3193	1/1	0.97	0.44	20,20,20,20	0
55	MG	2A	3072	1/1	0.97	0.30	39,39,39,39	0
55	MG	2A	3282	1/1	0.97	0.16	41,41,41,41	0
55	MG	27	101	1/1	0.97	0.68	38,38,38,38	0
55	MG	1A	3818	1/1	0.97	0.15	40,40,40,40	0
55	MG	28	101	1/1	0.97	0.82	36,36,36,36	0
55	MG	2A	3530	1/1	0.97	0.29	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	2A	3787	1/1	0.97	0.13	20,20,20,20	0
55	MG	1A	3819	1/1	0.97	0.05	23,23,23,23	0
55	MG	2A	3076	1/1	0.97	0.39	36,36,36,36	0
55	MG	1A	3820	1/1	0.97	0.06	53,53,53,53	0
55	MG	2A	3287	1/1	0.97	0.12	24,24,24,24	0
55	MG	1A	3597	1/1	0.97	0.30	67,67,67,67	0
55	MG	1A	3281	1/1	0.97	0.09	58,58,58,58	0
55	MG	2A	3290	1/1	0.97	0.14	29,29,29,29	0
55	MG	1A	3282	1/1	0.97	0.09	18,18,18,18	0
55	MG	2A	3292	1/1	0.97	0.07	38,38,38,38	0
55	MG	2a	1608	1/1	0.97	0.20	88,88,88,88	0
55	MG	1A	3338	1/1	0.97	0.10	17,17,17,17	0
55	MG	1A	3705	1/1	0.97	0.13	58,58,58,58	0
55	MG	1B	216	1/1	0.97	0.09	29,29,29,29	0
55	MG	2A	3088	1/1	0.97	0.66	44,44,44,44	0
55	MG	2A	3297	1/1	0.97	0.12	40,40,40,40	0
55	MG	1A	3194	1/1	0.97	0.17	39,39,39,39	0
55	MG	1B	218	1/1	0.97	0.15	51,51,51,51	0
55	MG	2A	3808	1/1	0.97	0.13	48,48,48,48	0
55	MG	2A	3547	1/1	0.97	0.05	50,50,50,50	0
55	MG	2A	3301	1/1	0.97	0.11	52,52,52,52	0
55	MG	1A	3508	1/1	0.97	0.07	46,46,46,46	0
55	MG	2A	3813	1/1	0.97	0.11	21,21,21,21	0
55	MG	1A	3423	1/1	0.97	0.14	9,9,9,9	0
55	MG	2A	3551	1/1	0.97	0.09	60,60,60,60	0
55	MG	1A	3837	1/1	0.97	0.12	9,9,9,9	0
55	MG	1A	3425	1/1	0.97	0.16	10,10,10,10	0
55	MG	1a	1784	1/1	0.97	0.21	74,74,74,74	0
55	MG	2A	3309	1/1	0.97	0.10	41,41,41,41	0
55	MG	2A	3310	1/1	0.97	0.05	69,69,69,69	0
55	MG	2A	3822	1/1	0.97	0.06	53,53,53,53	0
55	MG	1B	223	1/1	0.97	0.23	61,61,61,61	0
55	MG	2A	3824	1/1	0.97	0.18	47,47,47,47	0
55	MG	2A	3313	1/1	0.97	0.10	36,36,36,36	0
55	MG	2A	3826	1/1	0.97	0.05	43,43,43,43	0
55	MG	2A	3314	1/1	0.97	0.12	31,31,31,31	0
55	MG	1a	1787	1/1	0.97	0.06	60,60,60,60	0
55	MG	1A	3839	1/1	0.97	0.09	11,11,11,11	0
55	MG	1A	3340	1/1	0.97	0.10	20,20,20,20	0
55	MG	1A	3712	1/1	0.97	0.12	11,11,11,11	0
55	MG	1A	3250	1/1	0.97	0.12	44,44,44,44	0
55	MG	1A	3286	1/1	0.97	0.20	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1A	3432	1/1	0.97	0.20	8,8,8,8	0
55	MG	2A	3835	1/1	0.97	0.10	41,41,41,41	0
55	MG	2A	3323	1/1	0.97	0.19	27,27,27,27	0
55	MG	1A	3611	1/1	0.97	0.14	60,60,60,60	0
55	MG	1A	3220	1/1	0.97	0.81	27,27,27,27	0
55	MG	1A	3346	1/1	0.97	0.14	12,12,12,12	0
55	MG	2A	3840	1/1	0.97	0.14	39,39,39,39	0
55	MG	2A	3841	1/1	0.97	0.09	25,25,25,25	0
55	MG	2A	3327	1/1	0.97	0.13	34,34,34,34	0
55	MG	1A	3852	1/1	0.97	0.20	29,29,29,29	0
55	MG	2A	3329	1/1	0.97	0.10	43,43,43,43	0
55	MG	2a	1652	1/1	0.97	0.20	43,43,43,43	0
55	MG	2a	1653	1/1	0.97	0.26	70,70,70,70	0
55	MG	1a	1798	1/1	0.97	0.10	48,48,48,48	0
55	MG	1A	3028	1/1	0.97	0.39	19,19,19,19	0
55	MG	1a	1800	1/1	0.97	0.24	45,45,45,45	0
55	MG	1A	3437	1/1	0.97	0.07	9,9,9,9	0
55	MG	1A	3100	1/1	0.97	0.16	43,43,43,43	0
55	MG	2A	3851	1/1	0.97	0.17	66,66,66,66	0
55	MG	1a	1803	1/1	0.97	0.13	40,40,40,40	0
55	MG	2A	3582	1/1	0.97	0.12	29,29,29,29	0
55	MG	1A	3356	1/1	0.97	0.15	20,20,20,20	0
55	MG	1D	313	1/1	0.97	0.43	24,24,24,24	0
55	MG	2A	3338	1/1	0.97	0.17	51,51,51,51	0
55	MG	1A	3254	1/1	0.97	0.42	41,41,41,41	0
55	MG	2A	3859	1/1	0.97	0.30	62,62,62,62	0
55	MG	1a	1657	1/1	0.97	0.10	67,67,67,67	0
55	MG	2A	3588	1/1	0.97	0.18	24,24,24,24	0
55	MG	1A	3526	1/1	0.97	0.06	28,28,28,28	0
55	MG	1A	3726	1/1	0.97	0.12	44,44,44,44	0
55	MG	2A	3125	1/1	0.97	0.18	44,44,44,44	0
55	MG	1A	3441	1/1	0.97	0.16	16,16,16,16	0
55	MG	1A	3134	1/1	0.97	0.17	24,24,24,24	0
55	MG	1A	3531	1/1	0.97	0.08	42,42,42,42	0
55	MG	1A	3730	1/1	0.97	0.14	61,61,61,61	0
55	MG	2A	3349	1/1	0.97	0.11	42,42,42,42	0
55	MG	1A	3293	1/1	0.97	0.09	45,45,45,45	0
55	MG	2A	3352	1/1	0.97	0.09	48,48,48,48	0
55	MG	1a	1816	1/1	0.97	0.10	51,51,51,51	0
55	MG	2A	3355	1/1	0.97	0.05	54,54,54,54	0
55	MG	2A	3602	1/1	0.97	0.16	53,53,53,53	0
55	MG	2A	3135	1/1	0.97	0.17	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3533	1/1	0.97	0.09	25,25,25,25	0
55	MG	1A	3227	1/1	0.97	0.59	28,28,28,28	0
55	MG	1A	3295	1/1	0.97	0.08	18,18,18,18	0
55	MG	2A	3140	1/1	0.97	0.23	51,51,51,51	0
55	MG	1A	3628	1/1	0.97	0.14	10,10,10,10	0
55	MG	2A	3364	1/1	0.97	0.13	37,37,37,37	0
55	MG	2A	3610	1/1	0.97	0.13	35,35,35,35	0
55	MG	1a	1821	1/1	0.97	0.05	70,70,70,70	0
55	MG	1A	3147	1/1	0.97	0.71	30,30,30,30	0
55	MG	2A	3367	1/1	0.97	0.11	36,36,36,36	0
55	MG	2A	3614	1/1	0.97	0.04	62,62,62,62	0
55	MG	2A	3887	1/1	0.97	0.08	76,76,76,76	0
55	MG	2A	3144	1/1	0.97	0.62	33,33,33,33	0
55	MG	2A	3369	1/1	0.97	0.13	28,28,28,28	0
55	MG	1a	1823	1/1	0.97	0.24	51,51,51,51	0
55	MG	2A	3371	1/1	0.97	0.08	45,45,45,45	0
55	MG	1A	3874	1/1	0.97	0.07	27,27,27,27	0
55	MG	1A	3365	1/1	0.97	0.07	33,33,33,33	0
55	MG	1F	309	1/1	0.97	0.57	21,21,21,21	0
55	MG	2A	3375	1/1	0.97	0.10	21,21,21,21	0
55	MG	1a	1827	1/1	0.97	0.08	49,49,49,49	0
55	MG	1A	3449	1/1	0.97	0.11	45,45,45,45	0
55	MG	1F	311	1/1	0.97	0.37	11,11,11,11	0
55	MG	1A	3366	1/1	0.97	0.08	27,27,27,27	0
55	MG	1A	3740	1/1	0.97	0.12	46,46,46,46	0
55	MG	2A	3904	1/1	0.97	0.14	35,35,35,35	0
55	MG	2A	3382	1/1	0.97	0.11	37,37,37,37	0
55	MG	1A	3741	1/1	0.97	0.73	29,29,29,29	0
55	MG	1A	3540	1/1	0.97	0.22	32,32,32,32	0
55	MG	1A	3298	1/1	0.97	0.08	34,34,34,34	0
55	MG	2A	3910	1/1	0.97	0.19	37,37,37,37	0
55	MG	2A	3157	1/1	0.97	0.15	51,51,51,51	0
55	MG	2A	3387	1/1	0.97	0.13	35,35,35,35	0
55	MG	1A	3181	1/1	0.97	0.48	34,34,34,34	0
55	MG	2A	3914	1/1	0.97	0.22	57,57,57,57	0
55	MG	1A	3745	1/1	0.97	0.14	28,28,28,28	0
55	MG	1A	3370	1/1	0.97	0.06	45,45,45,45	0
55	MG	2A	3162	1/1	0.97	0.20	33,33,33,33	0
55	MG	2A	3163	1/1	0.97	0.54	38,38,38,38	0
55	MG	1N	201	1/1	0.97	0.17	39,39,39,39	0
55	MG	1A	3545	1/1	0.97	0.11	40,40,40,40	0
55	MG	2a	1729	1/1	0.97	0.33	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3642	1/1	0.97	0.51	29,29,29,29	0
55	MG	2A	3167	1/1	0.97	0.20	35,35,35,35	0
55	MG	1A	3302	1/1	0.97	0.19	43,43,43,43	0
55	MG	2A	3400	1/1	0.97	0.08	29,29,29,29	0
55	MG	2A	3401	1/1	0.97	0.14	36,36,36,36	0
55	MG	1a	1687	1/1	0.97	0.12	31,31,31,31	0
55	MG	1P	203	1/1	0.97	0.68	9,9,9,9	0
55	MG	2A	3172	1/1	0.97	0.20	54,54,54,54	0
55	MG	1A	3644	1/1	0.97	0.09	30,30,30,30	0
55	MG	1Q	202	1/1	0.97	0.11	19,19,19,19	0
55	MG	2A	3407	1/1	0.97	0.12	32,32,32,32	0
55	MG	1b	3001	1/1	0.97	0.06	79,79,79,79	0
55	MG	1A	3304	1/1	0.97	0.10	34,34,34,34	0
55	MG	2A	3657	1/1	0.97	0.16	45,45,45,45	0
55	MG	1A	3373	1/1	0.97	0.11	7,7,7,7	0
55	MG	1A	3647	1/1	0.97	0.13	28,28,28,28	0
55	MG	1T	201	1/1	0.97	0.10	30,30,30,30	0
55	MG	1A	3896	1/1	0.97	0.12	35,35,35,35	0
55	MG	2A	3416	1/1	0.97	0.12	21,21,21,21	0
55	MG	1A	3305	1/1	0.97	0.11	47,47,47,47	0
55	MG	1a	1698	1/1	0.97	0.07	37,37,37,37	0
55	MG	2A	3947	1/1	0.97	0.17	33,33,33,33	0
55	MG	2A	3665	1/1	0.97	0.13	38,38,38,38	0
55	MG	1A	3376	1/1	0.97	0.13	26,26,26,26	0
55	MG	1U	203	1/1	0.97	0.14	32,32,32,32	0
55	MG	1a	1703	1/1	0.97	0.16	42,42,42,42	0
55	MG	1A	3379	1/1	0.97	0.14	13,13,13,13	0
55	MG	2A	3953	1/1	0.97	0.38	48,48,48,48	0
55	MG	1A	3465	1/1	0.97	0.05	48,48,48,48	0
55	MG	2A	3427	1/1	0.97	0.20	44,44,44,44	0
55	MG	2a	1760	1/1	0.97	0.10	52,52,52,52	0
55	MG	1A	3088	1/1	0.97	0.68	24,24,24,24	0
55	MG	2A	3430	1/1	0.97	0.07	71,71,71,71	0
55	MG	2A	3189	1/1	0.97	0.48	43,43,43,43	0
55	MG	1a	1707	1/1	0.97	0.17	54,54,54,54	0
55	MG	2A	3435	1/1	0.97	0.13	42,42,42,42	0
55	MG	1A	3554	1/1	0.97	0.15	56,56,56,56	0
55	MG	1a	1709	1/1	0.97	0.09	37,37,37,37	0
55	MG	1t	3001	1/1	0.97	0.28	69,69,69,69	0
55	MG	1A	3310	1/1	0.97	0.16	17,17,17,17	0
55	MG	2A	3002	1/1	0.97	0.13	38,38,38,38	0
55	MG	1A	3468	1/1	0.97	0.17	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3906	1/1	0.97	0.08	14,14,14,14	0
55	MG	2A	3686	1/1	0.97	0.15	39,39,39,39	0
55	MG	1A	3136	1/1	0.97	0.24	31,31,31,31	0
55	MG	1A	3471	1/1	0.97	0.09	46,46,46,46	0
55	MG	2A	3445	1/1	0.97	0.12	55,55,55,55	0
55	MG	2A	3446	1/1	0.97	0.16	22,22,22,22	0
55	MG	2B	3004	1/1	0.97	0.20	67,67,67,67	0
55	MG	1A	3659	1/1	0.97	0.12	6,6,6,6	0
55	MG	1A	3312	1/1	0.97	0.10	36,36,36,36	0
55	MG	1A	3769	1/1	0.97	0.04	30,30,30,30	0
55	MG	1A	3474	1/1	0.97	0.97	18,18,18,18	0
55	MG	1A	3913	1/1	0.97	0.21	27,27,27,27	0
55	MG	1A	3387	1/1	0.97	0.04	54,54,54,54	0
55	MG	2A	3453	1/1	0.97	0.11	36,36,36,36	0
55	MG	2A	3208	1/1	0.97	0.11	38,38,38,38	0
55	MG	2A	3700	1/1	0.97	0.14	58,58,58,58	0
55	MG	2A	3455	1/1	0.97	0.32	62,62,62,62	0
55	MG	2A	3209	1/1	0.97	0.58	36,36,36,36	0
55	MG	1A	3773	1/1	0.97	0.10	20,20,20,20	0
55	MG	2A	3018	1/1	0.97	0.28	41,41,41,41	0
55	MG	1A	3035	1/1	0.97	0.11	16,16,16,16	0
55	MG	1A	3666	1/1	0.97	0.10	42,42,42,42	0
55	MG	2B	3021	1/1	0.97	0.09	45,45,45,45	0
55	MG	2B	3022	1/1	0.97	0.33	68,68,68,68	0
55	MG	2A	3216	1/1	0.97	0.29	37,37,37,37	0
55	MG	1A	3167	1/1	0.97	0.54	33,33,33,33	0
55	MG	2A	3464	1/1	0.97	0.14	37,37,37,37	0
55	MG	2A	3465	1/1	0.97	0.08	32,32,32,32	0
55	MG	1A	3206	1/1	0.97	0.34	18,18,18,18	0
55	MG	2A	3467	1/1	0.97	0.17	30,30,30,30	0
55	MG	2A	3715	1/1	0.97	0.06	37,37,37,37	0
55	MG	1A	3318	1/1	0.97	0.09	9,9,9,9	0
55	MG	1A	3207	1/1	0.97	0.60	27,27,27,27	0
55	MG	1A	3113	1/1	0.97	0.14	21,21,21,21	0
55	MG	1A	3210	1/1	0.97	0.38	28,28,28,28	0
55	MG	1A	3928	1/1	0.97	0.64	33,33,33,33	0
55	MG	1A	3483	1/1	0.97	0.10	62,62,62,62	0
55	MG	1a	1735	1/1	0.97	0.08	41,41,41,41	0
55	MG	2A	3475	1/1	0.97	0.24	39,39,39,39	0
55	MG	1A	3930	1/1	0.97	0.54	36,36,36,36	0
55	MG	1A	3114	1/1	0.97	0.36	18,18,18,18	0
55	MG	2A	3478	1/1	0.97	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	2A	3479	1/1	0.97	0.09	53,53,53,53	0
55	MG	1A	3212	1/1	0.97	0.32	21,21,21,21	0
55	MG	1A	3785	1/1	0.97	0.14	8,8,8,8	0
55	MG	2A	3237	1/1	0.97	0.17	41,41,41,41	0
55	MG	2A	3240	1/1	0.97	0.41	37,37,37,37	0
55	MG	1A	3153	1/1	0.97	0.82	26,26,26,26	0
55	MG	2a	1824	1/1	0.97	0.59	65,65,65,65	0
55	MG	2A	3486	1/1	0.97	0.33	59,59,59,59	0
55	MG	1A	3936	1/1	0.97	0.12	41,41,41,41	0
55	MG	1A	3487	1/1	0.97	0.16	21,21,21,21	0
55	MG	2F	304	1/1	0.97	0.60	45,45,45,45	0
55	MG	2A	3489	1/1	0.97	0.34	38,38,38,38	0
55	MG	2A	3244	1/1	0.97	0.52	29,29,29,29	0
55	MG	2F	307	1/1	0.97	0.09	30,30,30,30	0
55	MG	1A	3326	1/1	0.97	0.07	32,32,32,32	0
55	MG	1A	3407	1/1	0.97	0.38	34,34,34,34	0
55	MG	1A	3582	1/1	0.97	0.34	14,14,14,14	0
55	MG	1A	3941	1/1	0.97	0.11	48,48,48,48	0
55	MG	2a	1837	1/1	0.97	0.17	51,51,51,51	0
55	MG	1A	3796	1/1	0.97	0.13	33,33,33,33	0
55	MG	2A	3496	1/1	0.97	0.10	43,43,43,43	0
55	MG	1A	3797	1/1	0.97	0.45	37,37,37,37	0
55	MG	1A	3684	1/1	0.97	0.24	41,41,41,41	0
55	MG	2A	3500	1/1	0.97	0.12	45,45,45,45	0
55	MG	1A	3095	1/1	0.97	0.28	21,21,21,21	0
55	MG	2A	3253	1/1	0.97	0.21	56,56,56,56	0
55	MG	1a	1607	1/1	0.97	0.06	74,74,74,74	0
55	MG	2A	3752	1/1	0.97	0.07	31,31,31,31	0
55	MG	1A	3491	1/1	0.97	0.10	21,21,21,21	0
55	MG	2Q	202	1/1	0.97	0.17	34,34,34,34	0
55	MG	2A	3256	1/1	0.97	0.52	45,45,45,45	0
55	MG	2Q	204	1/1	0.97	0.17	32,32,32,32	0
55	MG	2A	3755	1/1	0.97	0.27	35,35,35,35	0
55	MG	1A	3409	1/1	0.97	0.33	21,21,21,21	0
55	MG	1A	3410	1/1	0.97	0.15	8,8,8,8	0
55	MG	2A	3758	1/1	0.97	0.11	32,32,32,32	0
55	MG	2A	3759	1/1	0.97	0.15	28,28,28,28	0
55	MG	1A	3588	1/1	0.97	0.79	31,31,31,31	0
55	MG	1A	3808	1/1	0.97	0.12	14,14,14,14	0
55	MG	1A	3952	1/1	0.97	0.43	23,23,23,23	0
55	MG	1A	3116	1/1	0.97	0.09	35,35,35,35	0
55	MG	2U	204	1/1	0.97	0.50	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3694	1/1	0.97	0.14	31,31,31,31	0
55	MG	2V	201	1/1	0.97	0.25	40,40,40,40	0
55	MG	2A	3265	1/1	0.97	0.26	50,50,50,50	0
55	MG	2A	3266	1/1	0.97	0.53	41,41,41,41	0
55	MG	2A	3222	1/1	0.98	0.38	42,42,42,42	0
55	MG	1A	3829	1/1	0.98	0.15	50,50,50,50	0
55	MG	2A	3224	1/1	0.98	0.51	31,31,31,31	0
55	MG	1A	3342	1/1	0.98	0.08	30,30,30,30	0
55	MG	2A	3075	1/1	0.98	0.33	50,50,50,50	0
55	MG	2A	3391	1/1	0.98	0.35	63,63,63,63	0
55	MG	2A	3934	1/1	0.98	0.10	45,45,45,45	0
55	MG	2A	3227	1/1	0.98	0.41	49,49,49,49	0
55	MG	2A	3228	1/1	0.98	0.14	43,43,43,43	0
55	MG	2A	3229	1/1	0.98	0.10	29,29,29,29	0
55	MG	1A	3831	1/1	0.98	0.11	13,13,13,13	0
55	MG	1A	3235	1/1	0.98	0.10	27,27,27,27	0
55	MG	2A	3079	1/1	0.98	0.35	41,41,41,41	0
55	MG	1A	3576	1/1	0.98	0.12	13,13,13,13	0
55	MG	2A	3399	1/1	0.98	0.07	38,38,38,38	0
55	MG	2A	3943	1/1	0.98	0.19	38,38,38,38	0
55	MG	1A	3652	1/1	0.98	0.13	31,31,31,31	0
55	MG	1A	3835	1/1	0.98	0.10	14,14,14,14	0
55	MG	2A	3748	1/1	0.98	0.05	50,50,50,50	0
55	MG	1a	1812	1/1	0.98	0.07	50,50,50,50	0
55	MG	2A	3239	1/1	0.98	0.18	29,29,29,29	0
55	MG	2A	3084	1/1	0.98	0.53	38,38,38,38	0
55	MG	2A	3085	1/1	0.98	0.28	52,52,52,52	0
55	MG	1a	1692	1/1	0.98	0.21	53,53,53,53	0
55	MG	2A	3575	1/1	0.98	0.07	29,29,29,29	0
55	MG	1A	3836	1/1	0.98	0.09	27,27,27,27	0
55	MG	2A	3408	1/1	0.98	0.12	29,29,29,29	0
55	MG	2A	3578	1/1	0.98	0.29	43,43,43,43	0
55	MG	1A	3062	1/1	0.98	0.38	17,17,17,17	0
55	MG	1A	3289	1/1	0.98	0.12	24,24,24,24	0
55	MG	2A	3090	1/1	0.98	0.07	46,46,46,46	0
55	MG	1A	3450	1/1	0.98	0.09	63,63,63,63	0
55	MG	1A	3581	1/1	0.98	0.25	24,24,24,24	0
55	MG	2A	3414	1/1	0.98	0.10	70,70,70,70	0
55	MG	1A	3842	1/1	0.98	0.16	39,39,39,39	0
55	MG	1a	1699	1/1	0.98	0.09	33,33,33,33	0
55	MG	1A	3393	1/1	0.98	0.09	34,34,34,34	0
55	MG	1A	3452	1/1	0.98	0.18	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3394	1/1	0.98	0.10	18,18,18,18	0
55	MG	1A	3517	1/1	0.98	0.13	21,21,21,21	0
55	MG	2A	3099	1/1	0.98	0.22	43,43,43,43	0
55	MG	2A	3772	1/1	0.98	0.08	50,50,50,50	0
55	MG	2A	3422	1/1	0.98	0.07	60,60,60,60	0
55	MG	2B	3001	1/1	0.98	0.26	51,51,51,51	0
55	MG	2B	3002	1/1	0.98	0.05	69,69,69,69	0
55	MG	1A	3315	1/1	0.98	0.13	10,10,10,10	0
55	MG	2A	3424	1/1	0.98	0.12	72,72,72,72	0
55	MG	1A	3587	1/1	0.98	0.29	29,29,29,29	0
55	MG	2A	3426	1/1	0.98	0.07	66,66,66,66	0
55	MG	1B	201	1/1	0.98	0.45	27,27,27,27	0
55	MG	1A	3746	1/1	0.98	0.10	48,48,48,48	0
55	MG	2A	3429	1/1	0.98	0.14	23,23,23,23	0
55	MG	2A	3600	1/1	0.98	0.21	29,29,29,29	0
55	MG	1A	3851	1/1	0.98	0.14	43,43,43,43	0
55	MG	2B	3012	1/1	0.98	0.07	56,56,56,56	0
55	MG	2A	3431	1/1	0.98	0.20	20,20,20,20	0
55	MG	1A	3068	1/1	0.98	0.50	33,33,33,33	0
55	MG	2A	3107	1/1	0.98	0.43	40,40,40,40	0
55	MG	1a	1712	1/1	0.98	0.19	83,83,83,83	0
55	MG	2A	3264	1/1	0.98	0.23	16,16,16,16	0
55	MG	2a	1710	1/1	0.98	0.20	49,49,49,49	0
55	MG	2a	1712	1/1	0.98	0.18	59,59,59,59	0
55	MG	1A	3351	1/1	0.98	0.14	11,11,11,11	0
55	MG	1A	3352	1/1	0.98	0.12	11,11,11,11	0
55	MG	2a	1715	1/1	0.98	0.07	44,44,44,44	0
55	MG	2A	3267	1/1	0.98	0.49	44,44,44,44	0
55	MG	2A	3792	1/1	0.98	0.12	51,51,51,51	0
55	MG	2A	3793	1/1	0.98	0.04	52,52,52,52	0
55	MG	1A	3399	1/1	0.98	0.06	30,30,30,30	0
55	MG	1A	3353	1/1	0.98	0.10	13,13,13,13	0
55	MG	1A	3524	1/1	0.98	0.26	24,24,24,24	0
55	MG	2A	3797	1/1	0.98	0.12	36,36,36,36	0
55	MG	2D	301	1/1	0.98	0.30	46,46,46,46	0
55	MG	1A	3859	1/1	0.98	0.06	35,35,35,35	0
55	MG	2a	1725	1/1	0.98	0.19	58,58,58,58	0
55	MG	1A	3594	1/1	0.98	0.25	16,16,16,16	0
55	MG	1A	3525	1/1	0.98	0.14	33,33,33,33	0
55	MG	2A	3616	1/1	0.98	0.55	35,35,35,35	0
55	MG	2A	3117	1/1	0.98	0.27	36,36,36,36	0
55	MG	1B	214	1/1	0.98	0.06	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3404	1/1	0.98	0.06	38,38,38,38	0
55	MG	1A	3674	1/1	0.98	0.06	27,27,27,27	0
55	MG	1A	3354	1/1	0.98	0.09	12,12,12,12	0
55	MG	2A	3807	1/1	0.98	0.11	55,55,55,55	0
55	MG	1A	3676	1/1	0.98	0.05	25,25,25,25	0
55	MG	2A	3281	1/1	0.98	0.08	56,56,56,56	0
55	MG	2A	3810	1/1	0.98	0.10	27,27,27,27	0
55	MG	1a	1726	1/1	0.98	0.04	68,68,68,68	0
55	MG	1A	3355	1/1	0.98	0.04	10,10,10,10	0
55	MG	1A	3529	1/1	0.98	0.13	34,34,34,34	0
55	MG	1A	3868	1/1	0.98	0.12	29,29,29,29	0
55	MG	2A	3127	1/1	0.98	0.32	29,29,29,29	0
55	MG	1A	3600	1/1	0.98	0.35	41,41,41,41	0
55	MG	1A	3530	1/1	0.98	0.11	53,53,53,53	0
55	MG	1A	3042	1/1	0.98	0.54	1,1,1,1	0
55	MG	1A	3682	1/1	0.98	0.18	39,39,39,39	0
55	MG	1A	3319	1/1	0.98	0.06	52,52,52,52	0
55	MG	2A	3821	1/1	0.98	0.05	46,46,46,46	0
55	MG	2A	3463	1/1	0.98	0.16	36,36,36,36	0
55	MG	1A	3111	1/1	0.98	0.15	29,29,29,29	0
55	MG	2A	3136	1/1	0.98	0.13	34,34,34,34	0
55	MG	2F	308	1/1	0.98	0.68	34,34,34,34	0
55	MG	2A	3637	1/1	0.98	0.23	39,39,39,39	0
55	MG	1A	3469	1/1	0.98	0.19	41,41,41,41	0
55	MG	1A	3045	1/1	0.98	0.12	13,13,13,13	0
55	MG	1D	302	1/1	0.98	0.21	22,22,22,22	0
55	MG	1A	3123	1/1	0.98	0.37	24,24,24,24	0
55	MG	1A	3688	1/1	0.98	0.13	23,23,23,23	0
55	MG	1D	305	1/1	0.98	0.13	42,42,42,42	0
55	MG	1A	3225	1/1	0.98	0.10	25,25,25,25	0
55	MG	1a	1625	1/1	0.98	0.25	54,54,54,54	0
55	MG	2A	3646	1/1	0.98	0.21	40,40,40,40	0
55	MG	1A	3362	1/1	0.98	0.29	38,38,38,38	0
55	MG	1A	3363	1/1	0.98	0.06	19,19,19,19	0
55	MG	1A	3693	1/1	0.98	0.10	20,20,20,20	0
55	MG	2A	3307	1/1	0.98	0.09	57,57,57,57	0
55	MG	2A	3003	1/1	0.98	0.20	34,34,34,34	0
55	MG	1A	3296	1/1	0.98	0.11	36,36,36,36	0
55	MG	2A	3480	1/1	0.98	0.06	39,39,39,39	0
55	MG	1A	3416	1/1	0.98	0.07	38,38,38,38	0
55	MG	1A	3542	1/1	0.98	0.14	49,49,49,49	0
55	MG	2R	203	1/1	0.98	0.12	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3844	1/1	0.98	0.20	65,65,65,65	0
55	MG	1A	3076	1/1	0.98	0.26	17,17,17,17	0
55	MG	1A	3168	1/1	0.98	0.12	31,31,31,31	0
55	MG	1A	3889	1/1	0.98	0.35	34,34,34,34	0
55	MG	1A	3299	1/1	0.98	0.10	28,28,28,28	0
55	MG	1E	301	1/1	0.98	0.13	9,9,9,9	0
55	MG	1A	3300	1/1	0.98	0.09	21,21,21,21	0
55	MG	1A	3421	1/1	0.98	0.21	29,29,29,29	0
55	MG	2A	3014	1/1	0.98	0.15	23,23,23,23	0
55	MG	2A	3853	1/1	0.98	0.09	53,53,53,53	0
55	MG	2V	202	1/1	0.98	0.40	37,37,37,37	0
55	MG	2A	3015	1/1	0.98	0.50	44,44,44,44	0
55	MG	2A	3161	1/1	0.98	0.22	31,31,31,31	0
55	MG	2A	3666	1/1	0.98	0.14	51,51,51,51	0
55	MG	2A	3016	1/1	0.98	0.50	38,38,38,38	0
55	MG	1a	1639	1/1	0.98	0.13	63,63,63,63	0
55	MG	1A	3894	1/1	0.98	0.06	13,13,13,13	0
55	MG	1A	3895	1/1	0.98	0.06	21,21,21,21	0
55	MG	2A	3671	1/1	0.98	0.05	52,52,52,52	0
55	MG	1A	3369	1/1	0.98	0.11	12,12,12,12	0
55	MG	2A	3021	1/1	0.98	0.68	44,44,44,44	0
55	MG	2A	3499	1/1	0.98	0.29	28,28,28,28	0
55	MG	20	103	1/1	0.98	0.11	64,64,64,64	0
55	MG	1A	3261	1/1	0.98	0.16	20,20,20,20	0
55	MG	1A	3898	1/1	0.98	0.08	58,58,58,58	0
55	MG	2I	8001	1/1	0.98	0.07	51,51,51,51	0
55	MG	1A	3424	1/1	0.98	0.09	45,45,45,45	0
55	MG	1A	3790	1/1	0.98	0.06	36,36,36,36	0
55	MG	1A	3097	1/1	0.98	0.44	23,23,23,23	0
55	MG	2A	3028	1/1	0.98	0.59	38,38,38,38	0
55	MG	1A	3303	1/1	0.98	0.15	27,27,27,27	0
55	MG	1a	1767	1/1	0.98	0.05	78,78,78,78	0
55	MG	1A	3794	1/1	0.98	0.07	50,50,50,50	0
55	MG	1A	3795	1/1	0.98	0.19	27,27,27,27	0
55	MG	1A	3707	1/1	0.98	0.08	33,33,33,33	0
55	MG	1A	3157	1/1	0.98	0.12	21,21,21,21	0
55	MG	2A	3035	1/1	0.98	0.10	41,41,41,41	0
55	MG	1A	3430	1/1	0.98	0.14	29,29,29,29	0
55	MG	1A	3334	1/1	0.98	0.19	29,29,29,29	0
55	MG	2A	3345	1/1	0.98	0.13	21,21,21,21	0
55	MG	1A	3629	1/1	0.98	0.09	55,55,55,55	0
55	MG	1A	3630	1/1	0.98	0.09	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3693	1/1	0.98	0.07	37,37,37,37	0
55	MG	2a	1816	1/1	0.98	0.41	66,66,66,66	0
55	MG	1A	3375	1/1	0.98	0.16	24,24,24,24	0
55	MG	2a	1818	1/1	0.98	0.16	45,45,45,45	0
55	MG	1A	3803	1/1	0.98	0.06	46,46,46,46	0
55	MG	1A	3492	1/1	0.98	0.19	28,28,28,28	0
55	MG	2a	1821	1/1	0.98	0.06	46,46,46,46	0
55	MG	1A	3806	1/1	0.98	0.09	37,37,37,37	0
55	MG	2a	1823	1/1	0.98	0.05	94,94,94,94	0
55	MG	2A	3045	1/1	0.98	0.12	28,28,28,28	0
55	MG	1A	3807	1/1	0.98	0.08	20,20,20,20	0
55	MG	2A	3890	1/1	0.98	0.23	43,43,43,43	0
55	MG	1A	3633	1/1	0.98	0.07	40,40,40,40	0
55	MG	2A	3357	1/1	0.98	0.10	23,23,23,23	0
55	MG	1A	3433	1/1	0.98	0.08	22,22,22,22	0
55	MG	1A	3919	1/1	0.98	0.14	9,9,9,9	0
55	MG	2A	3360	1/1	0.98	0.12	26,26,26,26	0
55	MG	1A	3283	1/1	0.98	0.13	9,9,9,9	0
55	MG	1A	3495	1/1	0.98	0.24	33,33,33,33	0
55	MG	2A	3898	1/1	0.98	0.09	24,24,24,24	0
55	MG	1a	1786	1/1	0.98	0.04	69,69,69,69	0
55	MG	1A	3377	1/1	0.98	0.14	16,16,16,16	0
55	MG	1R	201	1/1	0.98	0.17	20,20,20,20	0
55	MG	1R	202	1/1	0.98	0.11	26,26,26,26	0
55	MG	2A	3711	1/1	0.98	0.07	51,51,51,51	0
55	MG	2a	1841	1/1	0.98	0.07	87,87,87,87	0
55	MG	2A	3905	1/1	0.98	0.09	51,51,51,51	0
55	MG	2A	3712	1/1	0.98	0.06	44,44,44,44	0
55	MG	1A	3378	1/1	0.98	0.17	17,17,17,17	0
55	MG	1A	3924	1/1	0.98	0.21	16,16,16,16	0
55	MG	1A	3306	1/1	0.98	0.04	31,31,31,31	0
55	MG	2A	3716	1/1	0.98	0.11	27,27,27,27	0
55	MG	2A	3060	1/1	0.98	0.33	26,26,26,26	0
55	MG	1A	3926	1/1	0.98	0.04	52,52,52,52	0
55	MG	1A	3337	1/1	0.98	0.18	25,25,25,25	0
55	MG	1A	3641	1/1	0.98	0.30	36,36,36,36	0
55	MG	2A	3210	1/1	0.98	0.41	37,37,37,37	0
55	MG	1A	3382	1/1	0.98	0.12	35,35,35,35	0
55	MG	1A	3158	1/1	0.98	0.13	28,28,28,28	0
55	MG	1A	3309	1/1	0.98	0.14	7,7,7,7	0
55	MG	1A	3024	1/1	0.98	0.12	19,19,19,19	0
55	MG	1A	3569	1/1	0.98	0.09	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1V	203	1/1	0.98	0.17	29,29,29,29	0
55	MG	1A	3107	1/1	0.98	0.42	20,20,20,20	0
55	MG	2a	1644	1/1	0.98	0.27	46,46,46,46	0
56	ZN	1Y	501	1/1	0.98	0.10	43,43,43,43	0
55	MG	2A	3219	1/1	0.98	0.20	68,68,68,68	0
56	ZN	15	104	1/1	0.98	0.08	37,37,37,37	0
55	MG	1A	3827	1/1	0.98	0.12	57,57,57,57	0
55	MG	1A	3388	1/1	0.98	0.04	45,45,45,45	0
55	MG	2A	3926	1/1	0.98	0.11	50,50,50,50	0
56	ZN	29	103	1/1	0.98	0.10	66,66,66,66	0
55	MG	2A	3927	1/1	0.98	0.22	28,28,28,28	0
55	MG	2A	3946	1/1	0.99	0.08	24,24,24,24	0
55	MG	1A	3401	1/1	0.99	0.11	21,21,21,21	0
55	MG	1A	3223	1/1	0.99	0.09	31,31,31,31	0
55	MG	2A	3196	1/1	0.99	0.17	29,29,29,29	0
55	MG	1A	3841	1/1	0.99	0.06	20,20,20,20	0
55	MG	1A	3496	1/1	0.99	0.08	40,40,40,40	0
55	MG	1A	3463	1/1	0.99	0.09	13,13,13,13	0
55	MG	1P	201	1/1	0.99	0.08	23,23,23,23	0
55	MG	2A	3379	1/1	0.99	0.14	15,15,15,15	0
55	MG	1P	202	1/1	0.99	0.22	17,17,17,17	0
55	MG	2A	3760	1/1	0.99	0.16	31,31,31,31	0
55	MG	1A	3788	1/1	0.99	0.08	25,25,25,25	0
55	MG	2A	3044	1/1	0.99	0.21	26,26,26,26	0
55	MG	1A	3017	1/1	0.99	0.32	9,9,9,9	0
55	MG	1Q	201	1/1	0.99	0.05	27,27,27,27	0
55	MG	1A	3205	1/1	0.99	0.10	14,14,14,14	0
55	MG	1A	3791	1/1	0.99	0.11	38,38,38,38	0
55	MG	1Q	204	1/1	0.99	0.15	28,28,28,28	0
55	MG	1B	213	1/1	0.99	0.15	21,21,21,21	0
55	MG	2A	3128	1/1	0.99	0.14	39,39,39,39	0
55	MG	1A	3572	1/1	0.99	0.19	34,34,34,34	0
55	MG	1A	3573	1/1	0.99	0.22	10,10,10,10	0
55	MG	2A	3053	1/1	0.99	0.23	37,37,37,37	0
55	MG	2A	3300	1/1	0.99	0.06	31,31,31,31	0
55	MG	1A	3614	1/1	0.99	0.42	32,32,32,32	0
55	MG	2A	3775	1/1	0.99	0.09	35,35,35,35	0
55	MG	2A	3215	1/1	0.99	0.34	38,38,38,38	0
55	MG	1A	3500	1/1	0.99	0.09	44,44,44,44	0
55	MG	23	101	1/1	0.99	0.25	56,56,56,56	0
55	MG	2A	3134	1/1	0.99	0.10	40,40,40,40	0
55	MG	2A	3305	1/1	0.99	0.10	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	1700	1/1	0.99	0.04	75,75,75,75	0
55	MG	1A	3316	1/1	0.99	0.02	36,36,36,36	0
55	MG	1A	3105	1/1	0.99	0.35	33,33,33,33	0
55	MG	1A	3381	1/1	0.99	0.13	19,19,19,19	0
55	MG	1A	3856	1/1	0.99	0.12	34,34,34,34	0
55	MG	1A	3578	1/1	0.99	0.25	26,26,26,26	0
55	MG	2A	3312	1/1	0.99	0.10	23,23,23,23	0
55	MG	1A	3917	1/1	0.99	0.18	23,23,23,23	0
55	MG	1A	3750	1/1	0.99	0.10	14,14,14,14	0
55	MG	2A	3315	1/1	0.99	0.18	25,25,25,25	0
55	MG	1A	3661	1/1	0.99	0.10	27,27,27,27	0
55	MG	1A	3662	1/1	0.99	0.06	36,36,36,36	0
55	MG	1a	1710	1/1	0.99	0.06	38,38,38,38	0
55	MG	1A	3021	1/1	0.99	0.21	26,26,26,26	0
55	MG	1A	3208	1/1	0.99	0.34	16,16,16,16	0
55	MG	1A	3805	1/1	0.99	0.04	34,34,34,34	0
55	MG	1A	3200	1/1	0.99	0.37	23,23,23,23	0
55	MG	1A	3066	1/1	0.99	0.40	23,23,23,23	0
55	MG	2a	1711	1/1	0.99	0.03	62,62,62,62	0
55	MG	2A	3234	1/1	0.99	0.11	29,29,29,29	0
55	MG	1A	3473	1/1	0.99	0.04	20,20,20,20	0
55	MG	1A	3386	1/1	0.99	0.12	18,18,18,18	0
55	MG	1A	3810	1/1	0.99	0.03	35,35,35,35	0
55	MG	2A	3899	1/1	0.99	0.05	29,29,29,29	0
55	MG	2D	302	1/1	0.99	0.37	28,28,28,28	0
55	MG	2A	3238	1/1	0.99	0.37	30,30,30,30	0
55	MG	1A	3087	1/1	0.99	0.08	30,30,30,30	0
55	MG	1D	308	1/1	0.99	0.46	27,27,27,27	0
55	MG	10	105	1/1	0.99	0.06	49,49,49,49	0
55	MG	2A	3078	1/1	0.99	0.14	44,44,44,44	0
55	MG	1A	3870	1/1	0.99	0.09	47,47,47,47	0
55	MG	1A	3273	1/1	0.99	0.14	21,21,21,21	0
55	MG	1A	3232	1/1	0.99	0.16	16,16,16,16	0
55	MG	1A	3933	1/1	0.99	0.12	17,17,17,17	0
55	MG	1A	3307	1/1	0.99	0.12	12,12,12,12	0
55	MG	2a	1831	1/1	0.99	0.22	67,67,67,67	0
55	MG	1A	3345	1/1	0.99	0.14	4,4,4,4	0
55	MG	1A	3447	1/1	0.99	0.08	29,29,29,29	0
55	MG	2A	3433	1/1	0.99	0.20	33,33,33,33	0
55	MG	1A	3765	1/1	0.99	0.05	38,38,38,38	0
55	MG	2A	3529	1/1	0.99	0.18	21,21,21,21	0
55	MG	1A	3516	1/1	0.99	0.15	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3079	1/1	0.99	0.21	36,36,36,36	0
55	MG	1A	3721	1/1	0.99	0.07	18,18,18,18	0
55	MG	2E	304	1/1	0.99	0.09	16,16,16,16	0
55	MG	1E	303	1/1	0.99	0.15	11,11,11,11	0
55	MG	2A	3170	1/1	0.99	0.36	48,48,48,48	0
55	MG	1A	3821	1/1	0.99	0.12	33,33,33,33	0
55	MG	1A	3942	1/1	0.99	0.20	10,10,10,10	0
55	MG	1A	3822	1/1	0.99	0.09	50,50,50,50	0
55	MG	1A	3260	1/1	0.99	0.13	10,10,10,10	0
55	MG	1A	3824	1/1	0.99	0.04	23,23,23,23	0
55	MG	2A	3351	1/1	0.99	0.22	22,22,22,22	0
55	MG	1A	3348	1/1	0.99	0.15	11,11,11,11	0
55	MG	1A	3771	1/1	0.99	0.16	20,20,20,20	0
55	MG	2A	3354	1/1	0.99	0.09	39,39,39,39	0
55	MG	1A	3234	1/1	0.99	0.05	66,66,66,66	0
55	MG	1A	3350	1/1	0.99	0.16	14,14,14,14	0
55	MG	2A	3024	1/1	0.99	0.09	31,31,31,31	0
55	MG	1A	3278	1/1	0.99	0.10	42,42,42,42	0
55	MG	1A	3222	1/1	0.99	0.25	30,30,30,30	0
55	MG	1A	3331	1/1	0.99	0.20	10,10,10,10	0
55	MG	1A	3427	1/1	0.99	0.08	16,16,16,16	0
55	MG	2A	3105	1/1	0.99	0.47	39,39,39,39	0
55	MG	1A	3892	1/1	0.99	0.16	27,27,27,27	0
55	MG	1A	3601	1/1	0.99	0.24	57,57,57,57	0
55	MG	1A	3400	1/1	0.99	0.06	35,35,35,35	0
55	MG	1A	3458	1/1	0.99	0.12	14,14,14,14	0
56	ZN	16	101	1/1	0.99	0.11	34,34,34,34	0
56	ZN	19	103	1/1	0.99	0.11	40,40,40,40	0
55	MG	2A	3190	1/1	0.99	0.19	35,35,35,35	0
55	MG	1A	3429	1/1	0.99	0.18	18,18,18,18	0
55	MG	1A	3689	1/1	0.99	0.11	20,20,20,20	0
56	ZN	25	105	1/1	0.99	0.06	51,51,51,51	0
56	ZN	26	101	1/1	0.99	0.08	57,57,57,57	0
55	MG	2A	3278	1/1	0.99	0.29	38,38,38,38	0
55	MG	1A	3460	1/1	0.99	0.15	16,16,16,16	0
57	SF4	1d	302	8/8	0.99	0.13	46,61,71,75	0
57	SF4	2d	501	8/8	0.99	0.14	54,68,91,93	0
55	MG	1A	3263	1/1	1.00	0.09	35,35,35,35	0
55	MG	1A	3850	1/1	1.00	0.24	43,43,43,43	0
55	MG	1A	3121	1/1	1.00	0.11	21,21,21,21	0
55	MG	1A	3180	1/1	1.00	0.20	24,24,24,24	0
55	MG	1A	3402	1/1	1.00	0.09	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3130	1/1	1.00	0.08	14,14,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.